

## TRI Relative Risk-Based Environmental Indicators Methodology

### **ERRATA**

The sorted compilation of toxicity weights for scored TRI chemicals found in Appendix C, Table C-1 has several omissions and errors. Since the toxicity weights for various TRI chemicals are undergoing further review, and modifications of the scores and the addition of new chemicals are likely, the reader should consult the most recent listing of the toxicity weights used in the TRI Environmental Indicators. Please contact the authors to obtain the most recently published listing.

**TOXICS RELEASE INVENTORY  
RELATIVE RISK-BASED  
ENVIRONMENTAL INDICATORS METHODOLOGY**

Nicolaas W. Bouwes, Ph.D.  
Steven M. Hassur, Ph.D.

Economics, Exposure and Technology Division  
Office of Pollution Prevention and Toxics  
U.S. Environmental Protection Agency

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Contractor Support:

Abt Associates, Inc.  
4800 Montgomery Lane  
Bethesda, MD 20814

For further information or inquiries, please contact:

Nicolaas W. Bouwes, Ph.D.  
(202) 260-1622  
bouwes.nick@epamail.epa.gov

or

Steven M. Hassur, Ph.D.  
(202) 260-1735  
hassur.steven@epamail.epa.gov

Economics, Exposure and Technology Division (7406)  
Office of Pollution Prevention and Toxics  
U.S. Environmental Protection Agency  
401 M St., SW  
Washington, D.C. 20460

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Project Managers: Nick Bouwes and Steve Hassur

### Work Group Members

Nicolaas Bouwes, Chair  
Steven Hassur  
Loren Hall  
Nancy Beach  
David Brooks  
Daniel Bushman  
Karen Hammerstrom  
Sondra Hollister  
John Leitzke  
Patrick Miller  
Samuel Sasnett  
Nestor Tirado  
Sylvon Vonderpool  
Andrew Wheeler

Thanks to these individuals for providing exposure-related support:

Bob Boethling  
David Lynch

### Abt Associates Project Staff

Susan Egan Keane, Project Manager  
Brad Firlie, Deputy Project Manager  
Lisa Akeson  
Amy Benson  
Kathy Cunningham  
Jonathan Kleinman  
Michael Müller  
Alexandra Varlay  
Carol Wagett  
Richard Walkling  
Richard Wells  
Michael Conti (technical reviewer)



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## EXECUTIVE SUMMARY

### INTRODUCTION

In 1989, EPA outlined the goals for establishing strategic planning processes at the Agency. Underlying this approach was the Agency's desire to set priorities and direct resources to areas with the greatest opportunity to achieve health and environmental risk reductions. As part of this initiative, the Administrator set forth a plan to develop indicators to track changes in environmental health impacts over time. Tracking these changes would allow the Agency to measure its progress in implementing environmental protection and pollution prevention programs. In addition, comparing the relative contribution of particular chemicals, industries and geographic regions through the indicators would allow the Agency (and other users) to establish priorities for improving future environmental health.

To efficiently track changes in human health and environmental impacts over time, the Agency would need to take advantage of existing data sources that reflect multimedia trends in environmental contaminant releases. The Toxics Release Inventory (TRI) is arguably one of the Agency's most relevant source of continuous data for developing indicators of change in environmental impacts over time. The TRI is mandated by the Emergency Planning and Community Right-to-Know Act (EPCRA) Title III Section 313 and requires that U.S. manufacturing facilities file annual reports documenting multimedia environmental releases and off-site transfers for over 606 chemicals and chemical categories which are of concern to the Agency. The Agency had recently added 286 new chemicals and chemical categories to the Section 313 list of toxic chemicals, effective for the reporting year 1995 (that is, the first reports on these chemicals were due on July 1, 1996) (59 *Federal Register* 61432, November 30, 1994). These additions have significantly expanded the scope of coverage of the TRI.

In response to the need for environmental indicators, and to take advantage of the rich data source offered by the TRI, the Office of Pollution Prevention and Toxics (OPPT) convened a workgroup that included members from several divisions within the Office, as well as individuals from other Agency Offices. The purpose of the workgroup was to explore the development of an indicator or indicators based on the TRI that could track changes in human health and environmental impacts better than reports of pounds of releases alone, specifically an approach that would integrate toxicity, exposure and population considerations into the evaluation of releases. This document presents the results of that effort, a method for developing TRI Relative Risk-based Environmental Indicators (referred to as "Indicators") plus additional developments and decisions that have transpired over time. The Indicators may eventually consist of a set of four indicators to separately track: (1) chronic human health, (2) acute human health, (3) chronic ecological and (4) acute ecological impacts. The focus of this report is the development of indicators of chronic human health impacts and aquatic life impacts; the development of corresponding acute effects indicators is not feasible now, since the data

to support such indicators are not available.<sup>1</sup> Furthermore, to the extent possible, the method is based on currently available, already-reviewed EPA approaches, data sets and models, in order to minimize duplication of effort and to maximize consistency with other Agency efforts to evaluate human health and environmental impacts.

This report explains how the proposed Indicators are constructed, and includes discussions of the conceptual methodology, data sources, and the computational approach. Since the Indicators are based on risk-related scores, the report discusses the similarities and distinctions between the *relative risk-based* approach of the Indicators method and conventional quantitative risk assessments. It also describes a PC-based, stand-alone computer model developed to allow users to compute the Chronic Human Health Indicator and to easily perform complex diagnostics of Indicator components, as well as subindicator calculations.

In developing the Indicators, many approaches to assessing and ranking the potential impact of chemicals were reviewed. Numerous techniques to score the relative significance of TRI chemicals and facilities have been and continue to be developed, underscoring the widespread need for such methods. One objective of this report is to explain the Indicators to a variety of agencies and groups that may wish to use or adapt the Indicators or the methodologies to their own needs. A related objective is to describe the benefits of the Indicators approach in terms of flexibility, power and utility as an analytical and strategic policy planning tool.

### **How Indicator Toxicity Weightings Differ from EPCRA Section 313 Statutory Criteria**

The TRI Relative Risk-Based Environmental Indicators utilize Toxics Release Inventory (TRI) chemical reporting data. All of the TRI chemicals included in the Indicators are listed on the TRI because they meet one or more statutory criteria regarding acute or chronic human toxicity, or environmental toxicity. The goal of the Indicators is to use data reported to the Agency to investigate the relative risk-based impacts of the releases and transfers of these chemicals on the general, non-worker population.

To do this, the Indicators must differentiate the relative toxicity of listed chemicals and rank them in a consistent manner. The ranking of each chemical reflects its toxicity only relative to other chemicals which are included in the Indicators; not to some benchmark or absolute value.

The TRI Relative Risk-Based Chronic Human Health Indicator addresses only the single, most sensitive chronic human health toxicity endpoint. Unlike the statutory criteria used for listing and delisting chemicals, the Chronic Human Health Indicator does not address the absolute chronic toxicity of chemicals on the TRI (e.g., multiple effects or the severity of effects); nor does it attempt to reflect the statutory criteria for these chemicals.

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<sup>1</sup>To appropriately evaluate potential acute effects, one would need to know the distribution of releases over time (peak release data), and these data are not currently reported through the TRI. However, possible future changes in reporting requirements may allow for the development of separate acute indicators for human and ecological effects.

It is important that the public not confuse the use of this Indicator as a screening-level tool for investigating relative risk-based impacts related to the releases and transfers of TRI chemicals, with the very different and separate activity of listing/delisting chemicals on the TRI using statutory criteria. The toxicity weightings provided in the Indicator method cannot be used as a scoring system for evaluating listing/delisting decisions.

#### *Emergency Planning and Community Right-to-Know Act Section 313 Statutory Criteria*

The Emergency Planning and Community Right-to-Know Act of 1986 (EPCRA) section 313(d)(2) sets out criteria for adding chemicals to the list of chemicals subject to reporting under EPCRA section 313(a). For a chemical (or category of chemicals) to be added to the EPCRA section 313(c) list of toxic chemicals, the Administrator must judge whether there is sufficient evidence to establish any one of the following:

Acute Human Toxicity §313(d)(2)(A) - The chemical is known to cause or can reasonably be anticipated to cause significant adverse acute human health effects at concentration levels that are reasonably likely to exist beyond facility site boundaries as a result of continuous, or frequently recurring, releases.

Chronic Human Toxicity §313(d)(2)(B) - The chemical is known to cause or can reasonably be anticipated to cause in humans—

- (i) cancer or teratogenic effects, or
- (ii) serious or irreversible—
  - (I) reproductive dysfunctions,
  - (II) neurological disorders,
  - (III) heritable genetic mutations, or
  - (IV) other chronic health effects.

Environmental Toxicity §313(d)(2)(C) - The chemical is known to cause or can reasonably be anticipated to cause, because of—

- (i) its toxicity,
- (ii) its toxicity and persistence in the environment, or
- (iii) its toxicity and tendency to bioaccumulate in the environment, significant adverse effect on the environment of sufficient seriousness, in the judgement of the Administrator, to warrant reporting under this section.

To remove a chemical from the section 313(c) list, the Administrator must determine that there is not sufficient evidence to establish any of the criteria described above as required by EPCRA section 313(d)(3).

The EPA examines all of the studies available for a chemical to decide if the chemical is capable of causing any of the adverse health effects or environmental toxicity in the criteria. Agency guidelines describe when a study shows such effects as cancer (EPA, 1986a), developmental toxicity (teratogenic effects) (EPA, 1991b), or heritable genetic mutations (EPA, 1986b). The review makes a qualitative judgment regarding the potential of each chemical to meet at least one of the criteria and the chemical is added to the list if this judgment is positive. If a chemical is on the list and it is not possible to make a positive judgment regarding any of the criteria, then the chemical can be removed. There is no correlation between the toxicity criteria and methodology used to make listing decisions under EPCRA section 313 and the methodology used to rank chemicals for the Indicators.

#### *Relative Toxicity Weighting of Chemicals in the TRI Relative Risk-Based Chronic Human Health Indicator*

In order to help the Agency make decisions, comparisons can be made among chemicals once they are listed under EPCRA section 313. The TRI Chronic Human Health Indicator is based on aspects of the adverse health effects (cancer and noncancer), as well as on exposure and population factors, to permit the chemicals to be ranked relative to one another. These aspects are available in public Agency-generated databases. Uncertainty reflecting the quality and adequacy of the data is incorporated into a toxicity weighting each chemical receives. The approach is intended to differentiate the relative toxicity of these chemicals in a uniform manner, provide a clear and reproducible scoring system based upon easily accessible and publicly available information, and utilize EPA consensus opinion to the greatest extent possible.

A complete discussion of the methods used in deriving the toxicity weightings for the Indicator, as well as the chemical-specific data summaries and scores, is provided in *TRI Relative Risk-based Environmental Indicators Project: Toxicity Weighting Summary Document* (EPA, 1997).

#### **GENERAL DESCRIPTION OF THE TRI RELATIVE RISK-BASED ENVIRONMENTAL INDICATORS**

This report describes the method for constructing the TRI Chronic Human Health Indicator and a draft method for the TRI Chronic Ecological Indicator. For both, the objective is to calculate a unitless value that reflects the overall risk-related impacts of releases and transfers of all included TRI chemicals from all reporting facilities to each environmental medium for a given year or years.

To construct Indicators that are related to risk, the reported quantity of TRI releases and transfers must be adjusted in a manner that relates to the risks associated with each media-specific release or transfer of each chemical. The risk potentially posed by a chemical release depends on the inherent toxicity of the chemical, the environmental fate and transport of the chemical in the medium to which it is released, the degree of contact between the contaminated medium and the human or ecological receptors, and the size of exposed population. Differences in these factors influence the relative contribution each release makes to each Indicator. Transfers to off-site locations such as sewage treatment plants (POTWs) require an additional estimate of the impact of treatment

technologies on the magnitude of releases. Such transfers are modeled based upon the exposure and population parameters associated with the off-site location.

In order to incorporate these factors into the Indicators, four main components are used to compute each Indicator. These are:

- the quantity of chemicals released or transferred,
- adjustments for chemical-specific toxicity,
- adjustments for pathway-specific exposure potential, and
- an adjustment to the Chronic Human Health Indicator to reflect size of the potentially exposed population.<sup>2,3</sup>

The TRI Chronic Human Health Indicator uses these components to perform a separate assessment for each unique combination of a chemical, facility, and release or transfer medium. Each of these releases or transfers results in a calculated Indicator “Element,” a unitless value proportional to the potential risk-based impact of each media-specific release or transfer. The value for the TRI Chronic Human Health Indicator is simply the sum of all the applicable Indicator Elements. Similarly, for the TRI Chronic Ecological Indicator, a separate assessment is made for each unique chemical-facility combination affecting the water medium, yielding the Ecological Indicator elements. The overall TRI Chronic Ecological Indicator is the sum of these elements.

The Indicators are calculated for each year in the TRI data set, beginning with 1988. These values can be compared in a number of ways. For example, one of the early years of TRI reporting, such as 1988, may be selected as the “base year” and later years’ Indicator values are compared to it. For the base year, the unitless score is scaled to 100,000; subsequent years’ data are scaled by the same factor to provide a relative comparison to the base year. This comparison allows assessment of the changes in estimated risk-related impacts of TRI releases and transfers from year to year.

Importantly, the Indicators can be aggregated or disaggregated in various ways, offering a vast number of possible combinations and views of the Indicators’ subcomponents. Each facility-chemical-media Indicator Element is retained by the computer program and thus can be evaluated by users wishing to investigate the structure of the Indicators. OPPT, other EPA Offices, Regions, States, or individuals could use these Indicator Elements to create their own queries that examine relative impacts from alternative perspectives, such as chemicals, industries, or geographic regions (among other parameters).

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<sup>2</sup>The method is focused on general populations: individuals, particularly highly exposed individuals, are not the focus of the Chronic Human Health Indicator. Furthermore, worker exposures are not addressed. Additional Indicators based upon highly exposed or sensitive subpopulations may be developed in the future.

<sup>3</sup>The Ecological Indicator does not consider populations.

The TRI Relative Risk-based Environmental Indicators method is not intended to be a quantitative risk assessment and does not calculate risk estimates. The method follows the same general paradigm often applied in quantitative assessments, but in a relative way. The Indicators are by their nature only intended to reflect the direction and the general magnitude of the change in releases over time, weighted by toxicity, exposure potential, and population factors that relate to potential risk. As such, an Indicator value has only relative rather than absolute meaning; it can only be used in comparisons to other Indicator values at different points in time, or in identifying the relative size of contributing factors to the overall Indicator.

Though this document presents conceptual methods for both the TRI Chronic Human Health Indicator and the TRI Chronic Ecological Indicator, the method is currently only being implemented for the Chronic Human Health Indicator. Further method development, and further data collection and analysis, will be required for the implementation of the TRI Chronic Ecological Indicator.

## **METHODS FOR CALCULATING TOXICITY WEIGHTS**

### **Chronic Human Toxicity Weights**

To weight a release based on potential toxicity, several factors could be considered, including the number of effects that the chemical causes, the relative severity of the effects it causes, the potency of the chemical for one or more of these effects, and the uncertainty associated with characterizing individual effects. The method used by the Indicators is patterned after EPA's Hazard Ranking System (HRS) (EPA, 1990b); this method focuses on the two latter factors. That is, toxicity scores are assigned based on quantitative potency data, with the additional consideration of a qualitative classification of the uncertainty (weight-of-evidence, or WOE) associated with data pertaining to carcinogenicity.

For this project, quantitative data on the human health effects on the TRI chemicals are compiled primarily from the Integrated Risk Information System (IRIS). Values available in IRIS include upper-bound cancer slope factor estimates ( $q_1^*$ ) or inhalation unit risk values for carcinogenic effects as well as Reference Doses (RfDs) or Reference Concentrations (RfCs) for noncancer effects. Data contained in IRIS have been peer-reviewed and represent Agency consensus. If IRIS data are not available, another source of toxicity data is the Health Effects Assessment Summary Tables (HEAST). These tables are constructed for use in both the Superfund program and in the RCRA program but do not represent Agency consensus. In cases where IRIS or HEAST do not have toxicity values and WOE classifications, several other sources for data were used to assign weights for use in the TRI Relative Risk-based Environmental Indicators method. Summaries of these other data, and suggested toxicity scores based on them, were provided for selected chemicals to a group of OPPT expert health scientists charged with reviewing toxicity data. After their review, this group then approved or disapproved the suggested scores through a disposition process. A complete discussion of the methods used in these evaluations, as well as the chemical-by-chemical data summaries and score assignments, are provided in *TRI Relative Risk-based Environmental Indicators Project: Toxicity Weighting Summary Document* (EPA, 1997).

The quantitative data is used in conjunction with qualitative weight-of-evidence information for carcinogenicity. The TRI Relative Risk-based Environmental Indicators method relies on categorical definitions from the EPA Guidelines for Carcinogen Risk Assessment (EPA, 1986a, currently being revised), which are related to the likelihood of a chemical's carcinogenicity in humans. For noncancer effects, since weight of evidence is considered in the development of quantitative toxicity values, the TRI Relative Risk-based Environmental Indicators method does not explicitly consider it again in assigning toxicity weights.

To assign toxicity weights to chemicals with carcinogenic effects, the TRI Relative Risk-based Environmental Indicators method uses a matrix to evaluate a chemical based on WOE and potency simultaneously. The columns of the matrix qualitatively classify chemicals with potential carcinogenic effects into two general WOE categories: known/probable (A/B) and possible (C). The rows of the matrix describe the ranges of slope factors considered. The particular ranges of slope factor values selected to represent each category correspond to the ranges presented in the HRS. The actual numerical weights assigned to the matrix cells correspond to the scores assigned in the HRS to these slope factor ranges. In certain cases, ranges presented in the matrix extend beyond those presented in the HRS because the range of slope factors for the TRI chemicals is broader than that covered by the HRS. The weights in the cells increase by an order of magnitude for each order of magnitude increase in slope factor and increase in the WOE category.

For chemicals with noncancer effects, toxicity weights are assigned based on the RfD. The actual values of the weights assigned are taken directly from the HRS, with the exception of the highest weighting category. The addition of an extra category was necessary because the RfD values for TRI chemicals extend beyond the ranges presented in the HRS.

The TRI Chronic Human Health Indicator weights a chemical based on the single most sensitive adverse effect for a given exposure pathway (either oral or inhalation). Inhalation and oral toxicity weights are developed separately. In general, if values are available for only one route, the same toxicity weight is applied for both routes. In rare instances, toxicity studies are available to show that a given chemical causes no health effects via one route; in these instances, the toxicity weight is assigned only to the route that results in effects. If a chemical exhibits both carcinogenic and noncarcinogenic effects, the higher of the associated cancer or noncancer weights is assigned as the final weight for the chemical for the given pathway. The method does not consider differences in the severity of the effects posed by the chemicals, nor does it adjust the weight if a chemical appears to demonstrate more than one adverse effect.

### **Chronic Ecological Toxicity Weights**

For ecological effects, the TRI Ecological Chronic Effects Indicator focuses on *aquatic* life impacts only. Very little data are available for most chemicals on effects to terrestrial or avian species; we assume the Chronic Human Health Indicator will provide some predictor of impacts on these species.

Aquatic toxicity weighting differs from human health toxicity weighting in two important respects. First, WOE is not considered a factor in the weighting scheme, since direct evidence of chemical toxicity is available from tests on aquatic species. Second, the aquatic toxicity weighting scheme simultaneously considers toxicity and bioaccumulation potential. Both of these measures are considered important when evaluating impacts on aquatic ecosystems.

Common numerical aquatic toxicity data include the Acute or Chronic Ambient Water Quality Criteria (AWQC), developed by the Office of Water, which may serve as the basis for water quality standards; the lethal concentration, 50 percent ( $LC_{50}$ ) - the chemical concentration in water at which 50 percent of test organisms die; and life-cycle or chronic No Observable Adverse Effect Levels (NOAELs). The measures of bioaccumulation potential that can be used are the bioconcentration factor (BCF) or bioaccumulation factor (BAF), the log of the octanol water partition coefficient ( $\log K_{ow}$ ), and the water solubility of the chemical.

The aquatic toxicity weight assigned to a chemical is a function of both its aquatic toxicity values and bioaccumulation potential values. Separate weights are assigned based on each of these measures; the chemical's final toxicity weight is the product of these individual weights.

## **METHODS FOR ADJUSTING RELEASES AND TRANSFERS FOR CHRONIC HUMAN EXPOSURE POTENTIAL**

Both qualitative and quantitative elements are considered when weighting chronic exposure potential. Quantitatively, generic exposure models are used to derive a "surrogate" dose level to characterize exposure potential on a exposure pathway-specific basis. Qualitatively, a level of uncertainty associated with the surrogate measures of exposure potential is assigned to each exposure pathway. The uncertainty estimates are then used to adjust the surrogate doses to derive the final exposure potential adjustment factor.

### **Quantitative Data Used in Evaluating Chronic Human Exposure Potential**

For the first step of deriving chronic exposure potential adjustment factors, quantitative measures of exposure potential must be estimated. In this methodology, comparisons across media can be made because a common quantitative exposure measure for each medium is derived, i.e., an estimate of "surrogate dose" — a measure related to the amount of chemical contacted by an individual per kilogram body weight per day.

To estimate the surrogate dose, a separate exposure evaluation is conducted for each media-specific emissions pathway (e.g., stack air, direct water, off-site transfer to landfills, etc.). In this methodology, the exposure evaluations combine data on media-specific and pathway-specific volumes, physicochemical properties and, where available, site characteristics; with models to determine an estimate of the ambient concentration of contaminant in the medium into which the chemical is released or transferred. The ambient media concentrations are then combined with standard human exposure assumptions to estimate the magnitude of the surrogate dose.

It must be emphasized that while this methodology uses the EPA exposure assessment paradigm to evaluate exposure potential, the results should not be construed as an actual numerical estimate of dose resulting from TRI releases, since limited facility-specific data and the use of generic models prevent the calculation of an actual dose. Instead, the purpose is to obtain an order of magnitude estimate of surrogate dose resulting from release of TRI chemicals *relative to the surrogate dose resulting from other releases included in the Indicator*, so that these releases can be weighted appropriately in the Indicator.

The exposure evaluation methods used for each type of release or transfer are specific to that type of release or transfer and depend on the models and data available to evaluate that emissions pathway. In some cases, models will be combined with some site-specific data to estimate exposure; in other cases, generic reasonable worst-case models may be used in the absence of any site-specific data.

### **Qualitative Data Used in Evaluating Chronic Human Exposure Potential**

Consideration of uncertainty in the exposure evaluation is necessary for making comparisons across emissions pathways, since the exposure evaluation methods for various pathways differ significantly in their level of refinement. For the purposes of calculating surrogate doses, the method defines uncertainty categories. The categories are defined so that surrogate dose estimates in a lower category are those more likely to overestimate exposure when compared to the next higher category and can correspondingly be adjusted. In general, surrogate dose estimates are placed in lower categories when they are developed using generic models and data that require many assumptions and extrapolations. These assumptions and extrapolations tend to be conservative, so that more generic modeling tends to yield overestimates of exposure. The initial surrogate dose estimate may be reduced by a factor of 5 or 10, depending on the uncertainty category to which it is assigned.

### **METHODS TO ADJUST FOR SIZE OF POPULATION EXPOSED**

The TRI Relative Risk-based Environmental Indicators method uses current 1990 U.S. Census data together with pathway-specific methods to estimate the size of exposed populations. The algorithms to determine the size of the population exposed to TRI releases vary substantially depending on the medium to which the chemical is released or transferred. The document discusses methods for estimating the size of the exposed population separately for each pathway.

For small populations, the method uses default numbers rather than absolute numbers to avoid undervaluing potentially high impacts on rural populations. Using default numbers assures small populations of a minimum weighting. In effect, this inclusion gives more weight per capita to small populations. For the air pathway, the Chronic Human Health Indicator method adjusts exposed populations below 1,000 persons to equal a value of 1,000. For the surface water pathway, the minimum population size is 10, while for groundwater, the minimum population size is 1.

Because of major difficulties in estimating sizes of the populations of ecological receptors, the TRI Ecological Indicator does not include a population weight. In effect, this approach assumes that all aquatic emissions occur in equally vulnerable locations. In actuality, the populations may differ among areas; thus, the Indicators method may either underestimate or overestimate impacts in a given area.

## COMPUTING THE TRI RELATIVE RISK-BASED ENVIRONMENTAL INDICATORS

To calculate the **Chronic Human Health Indicator**, the toxicity, exposure potential and population components are first combined multiplicatively to obtain a facility-chemical-medium specific element:

$$Indicator\ Element_{c,f,m} = Toxicity\ Weight_{c,m} \cdot Surrogate\ Dose_{c,f,m} \cdot ExposedPopulation_{f,m}$$

where:

c = subscript for chemical c,  
 f = subscript for facility f, and  
 m = subscript for medium m.

The components are multiplied because each component (toxicity, exposure, and population) contributes in a multiplicative way to the overall magnitude of the impact. The result of the multiplication of the components is a facility-chemical-medium-specific “Indicator Element.” It must be reiterated that this unitless element is *not* a physically meaningful measure of quantitative risk associated with the facility, but is a relative measure that is comparable to approximate measures for other facilities (or chemicals, media, etc.) calculated using the same methods.

For the **Chronic Ecological Indicator**, the following general equation combines toxicity and exposure potential components for each facility and for each chemical (only the water medium is evaluated):

$$Indicator\ Element_{c,f} = Toxicity\ Weight_c \cdot Surrogate\ Dose_{c,f}$$

where:

c = subscript for chemical c, and  
 f = subscript for facility f.

As with the Chronic Human Health Indicator, the components are multiplied in this setting because each component (toxicity and exposure) contributes multiplicatively to the overall magnitude of the impact. The result of the multiplication of the components is a facility-chemical-water-specific “Indicator Element.” The Elements should not be interpreted as actual quantitative measures of risk.

The method for calculating the Chronic Human Health Indicator and the Chronic Ecological Indicator is the same. Each is calculated by combining the individual TRI chemical-facility-media Indicator elements. A simple sum of the component values is used:

$$I = \sum \sum \sum IE_{c,f,m}$$

where:

I = TRI Relative Risk-based Environmental Indicator of interest and  
IE<sub>c,f,m</sub> = facility-chemical-medium-specific Indicator Element.

As many as 400,000 Indicator Elements for a given reporting year for the TRI will be summed to yield just one year's score for one of the TRI Relative Risk-based Environmental Indicators (e.g., the Chronic Human Health Indicator). In this method, each component score makes a contribution proportional to its size. The resulting Indicator Value can be used in a number of ways, including tracking changes over time. As noted earlier, the base-year Indicator is scaled to 100,000, and subsequent Indicators are scaled to this value to compare changes over time. It must be reiterated that while changes in scores over the years would imply that there have been changes in risk-based environmental impacts, the actual magnitude of any specific risk or change in risk is unknown in absolute terms.

### **Adjusting the Indicators for Changes in the TRI**

When a change occurs in the number of chemicals and facilities represented in TRI, the numerical value of the Indicators will almost certainly be altered if no adjustments are made to the method of calculation to account for the change. However, a difference in the Indicator value would not necessarily represent a sudden shift in actual environmental impact, but rather might reflect a broader understanding of the impacts that had existed all along. To maintain comparability in the Indicators' scores over time, the Indicators would have to be adjusted in some manner when such changes in the TRI occur.

A change in the number of chemicals and facilities in TRI can occur through several mechanisms. The addition to or deletion of chemicals from the TRI chemical list will occur as EPA responds to petitions or initiates its own action through the chemical listing or delisting process. Several additions and deletions to the dataset have already occurred since 1987, the first year of TRI reporting. Furthermore, as mentioned earlier, in November 1994 the Agency added 245 chemicals and chemical categories to the TRI chemical list, effective for the reporting year 1995. The deletion of chemicals would presumably have a minor effect since such chemicals would be deleted due to their low risk; these chemicals are likely to make only a minimal contribution to the Indicators.

Compliance with TRI reporting has changed over time, which had led to more facilities reporting. Increases in the number of reporting facilities may also occur as a result of changes in reporting requirements. For instance, in first two years of reporting, facilities that manufactured or

processed more than 50,000 pounds were required to report their releases. However, EPCRA lowered this threshold to 25,000 pounds in 1989. All of these modifications can act to alter the total emissions reported under TRI and the Indicator's estimate of the associated relative risk-based impacts.

To account for changes in the representation of chemicals and facilities in the TRI data base, the TRI Relative Risk-based Environmental Indicators method may create new Indicators when significant new additions are made to the TRI chemical list. "Significant" additions could be several minor additions that have been made over the course of a few years that eventually constitute a significant change, or a single major influx of new chemicals (due to Congressional or Agency action, for example). These new Indicators would include both old and new chemicals and facilities. However, to track trends for the initial set of chemicals and facilities, EPA would also retain a separate Indicator consisting of only the "original" facilities and chemicals.

While deletions from the chemical list of TRI chemicals probably would not result in any significant change to the Indicator value in most cases, the possibility of a change in value due solely to deletions makes adoption of adjustment methods important. Thus, when major deletions occur, the Indicator will be modified, excluding deleted chemicals, and then recomputed for all reporting years.

Finally, the yearly TRI data for a given chemical list of chemicals and facilities are the subject of ongoing quality control review and correction. As a result, yearly comparisons could be flawed if such revisions in reported data were not included in each previous year's Indicator. Therefore, the TRI Relative Risk-based Environmental Indicator will be recomputed for all years in the data base on an annual basis in order to incorporate revisions to the reporting data.

### **Generating "Subindicators"**

In addition to computing an overall Indicator value, the individual Indicator Elements can be combined in numerous other ways for further analysis. The detailed calculations used to create the Indicator Elements allow computation of "subindicators" for a wide variety of individual chemicals, geographic regions, industry sectors, facilities, exposure pathways and other parameters. These subindicators, like the overall Indicator, cannot be compared to some absolute level of concern, but can help identify the relative contribution of various components to the overall estimate of relative risk-based impacts of emissions. The ability of users to create these "subindicators" makes the TRI Relative Risk-based Environmental Indicators system a powerful tool for risk-based targeting, prioritization and strategic policy analysis.

## **CURRENT IMPLEMENTATION OF THE TRI RELATIVE RISK-BASED ENVIRONMENTAL INDICATORS METHOD**

### **Computer Program to Calculate the Indicators**

The TRI Chronic Human Health Indicator is currently implemented in a Microsoft Windows-based, stand alone, PC computer program. The program allows users to calculate the overall Chronic Human Health Indicator for all years of data and to present the results in various graphical and tabular formats, as well as save selected data to spreadsheet and data base formats (e.g., Microsoft Excel and dBase). The computer program also allows the users to create “subindicators” based upon specified parameters pertaining to the full complement of Indicator elements or upon selected subsets of reported data, or both of these approaches. The program includes on-line help for all of the program functions. A Users Guide will also be available.

### **Chemicals and Facilities Currently Included in the Indicators**

Conceptually, the Indicators method is intended to include all chemicals that are reportable to the Toxics Release Inventory. However, for the current version, some chemicals are excluded because they have not yet been assigned toxicity weights (many of these have had little or no reporting) or are missing physicochemical data. For the 1995 reporting year, there are 578 discrete chemicals and 28 separate chemical categories (including 39 additional chemicals in two delimited categories). In 1995, over 73,000 reports were filed from approximately 22,000 TRI facilities. Of these chemicals and chemical categories on the TRI List, 336 have been assigned toxicity scores; 288 of these are based on IRIS and HEAST values, and 48 based on expert review within OPPT. Scoring for all of the current TRI Indicators chemicals is discussed in the Interim Toxicity Weighting Summary Document (EPA, 1997) and is summarized in Appendix C of this document. For many chemicals that do not have toxicity scores, current reporting is zero. The evaluation of TRI chemicals with regard to aquatic toxicity will be conducted when the TRI Chronic Ecological Indicator is implemented.

## **ISSUES FOR FUTURE CONSIDERATION AND CONCLUSIONS**

There are two general types of issues to consider for future effort: specific methodological issues for the Indicators developed to date, and development of additional Indicators. The methodological questions associated with the Indicators developed to date include the following:

- how to compute the Acute Human Health and Acute Ecological Indicators given the current reporting under TRI;
- extending the Ecological Indicators beyond consideration of only aquatic life;

- whether severity of effect or multiple effects should be considered in the toxicity score for a chemical;
- for off-site transfers, how to better match TRI transfers to particular treatment practices (e.g., which TRI chemicals are sent to hazardous or nonhazardous waste management facilities; or which specific treatment practices are used at identified POTWs);
- how to incorporate information and/or estimates on changes in population for each year rather than using 1990 Census data for all years; and
- how to estimate the potential impact of non-landfill, non-incineration treatment (e.g., landfilling) or recycling.

The flexibility of the current TRI Relative Risk-based Environmental Indicators method and computer program allows accommodation of data from other sources besides the TRI data base. With additional data, the system could be used to develop additional Indicators that provide information on measures of environmental impacts other than risk alone. For example, Indicators that explicitly incorporate consideration of environmental justice issues could be developed using the Chronic Human Health Indicator as the foundation.

As an indication of improvements in environmental quality over time, the TRI Relative Risk-based Environmental Indicators will provide the EPA with a valuable tool to measure general trends based upon relative risk-related impacts of TRI chemicals. Though these Indicators do not capture all environmental releases of concern, they do generally relate changes in releases to relative changes in chronic human health and ecological (aquatic life) impacts from a large number of toxic chemicals of concern to the Agency. Importantly, the Indicators also provide an ability to analyze the relative contribution of chemicals and industrial sectors to environmental impacts, and serve as an analytical basis for setting priorities for pollution prevention, regulatory initiatives, enforcement targeting, and chemical testing.

## I. INTRODUCTION

In 1989, the EPA outlined the goals for establishing strategic planning processes at the Agency. Underlying this approach was the Agency's desire to set priorities and shift resources to areas with the greatest opportunity to achieve health and environmental risk reductions. As part of this initiative, the Administrator set forth a plan to develop indicators to track changes in environmental health impacts over time. Tracking these changes would allow the Agency to measure its progress in implementing environmental protection and pollution prevention programs. In addition, comparing the relative risk contribution of chemicals, industries and geographic regions through the indicators would allow the Agency (and other users) to establish priorities for improving environmental health.

Because one goal of such indicators is to allow EPA to track changes in human health and environmental impacts over time, the Agency would need to take advantage of existing data sources that reflect multimedia trends in environmental contaminant releases. One such database, the Toxics Release Inventory (TRI), is currently the Agency's most relevant source of continuous/regularly reported data for developing indicators of change in environmental impacts over time. The TRI is mandated by the Emergency Planning and Community Right-to-Know Act (EPCRA) Title III Section 313 and requires that U.S. manufacturing facilities file annual reports documenting multimedia environmental releases and off-site transfers for over 600 chemicals and chemical categories which are of concern to the Agency. The Agency had recently added 286 new chemicals and chemical categories to the Section 313 list of toxic chemicals, effective for the reporting year 1995 (that is, the first reports on these chemicals were due on July 1, 1996) (59 *Federal Register* 61432, November 30, 1994). These additions have significantly expanded the scope of coverage of the TRI.

In response to the need for environmental indicators, and to take advantage of the rich data source offered by the TRI, the Office of Pollution Prevention and Toxics (OPPT) convened a workgroup that included members from several divisions within the Office, as well as individuals from other Agency Offices. The purpose of the work group was to explore the development of an indicator or indicators based on the TRI that could track changes in human health and environmental impacts better than reports of pounds of releases alone.

In particular, the intent of the effort was to introduce a relative risk-based perspective in examining the trends in TRI reporting over time. When evaluating the local and community impacts of TRI chemicals, it is important to not only consider the number of pounds of a chemical released to the environment, but also the toxicity of the chemical, its exposure potential, and the size of the receptor population. The TRI Relative Risk-Based Environmental Indicators integrates these factors and provides a relative risk-based perspective of chemical releases and transfers.

This document presents the results of this effort, a method for developing TRI Relative Risk-based Environmental Indicators. The "TRI Relative Risk-based Environmental Indicators" may eventually consist of a set of four indicators to separately track: (1) chronic human health, (2) acute human health, (3) chronic ecological impacts and (4) acute ecological impacts. The focus of this

report is the development of meaningful indicators of chronic human health impacts and aquatic life impacts; the development of corresponding acute effects indicators is not feasible now, since the data to support such indicators are not available.<sup>1</sup> Furthermore, to the extent possible, the method presented is based on currently available, already-reviewed EPA approaches, data sets and models, in order to minimize duplication of effort and to maximize consistency with other Agency efforts to evaluate human health and environmental impacts.

This report explains how the proposed TRI Relative Risk-based Environmental Indicators are constructed, and includes discussions of the conceptual methodology, data sources, and the computational approach. Since the Indicators are based on risk-related scores, the report discusses the similarities and distinctions between the *relative risk-based* approach of the Indicators and conventional quantitative risk assessments. It also describes a PC-based, stand-alone computer model developed to allow users to compute the Chronic Human Health Indicator and to easily perform complex diagnostics of Indicator components, as well as subindicator calculations.

In developing the TRI Relative Risk-based Environmental Indicators, many approaches to assessing and ranking the potential impact of chemicals were reviewed. Numerous techniques to score the relative significance of TRI chemicals and facilities have been and continue to be developed, underscoring the widespread need for such methods. One objective of this report is to explain the Indicators to a variety of agencies and groups that may wish to use or adapt the Indicators or the methodologies to their own needs. A related objective is to describe the advantages of the Indicators approach in terms of flexibility, power and usefulness as an analytical and strategic policy planning tool.

This document was preceded by an earlier draft method document. The earlier document was described and released at a public meeting in September of 1992, and has been distributed to over 450 interested parties. It has received both internal and external review from a number of commenters. The current draft reflects a number of modifications to the original method, based on those comments and additional development work.

While the TRI database is the Agency's single best source of consistently reported release data, there are several limitations to any indicator that uses TRI data for tracking environmental health. The TRI data includes releases only from manufacturers in SIC codes 20-39 that employ more than ten full-time employees and manufacture or process more than 25,000 pounds or use more than 10,000 pounds of a chemical on the TRI chemical list. (In earlier years, the limitations were even broader.) Therefore, small manufacturers and many industrial sectors cannot be represented in a TRI-based indicator. Non-manufacturing activities for which releases are not required to be reported (but that may result in the emission of toxic chemicals) include dry cleaning, mining, the use and disposal of consumer products, the use of chemicals for agriculture, and operation of mobile

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<sup>1</sup>To appropriately evaluate potential acute effects, it is necessary to know the distribution of releases over time (peak release data), and these data are not currently reported through the TRI. However, possible future changes in reporting requirements may allow for the development of separate acute indicators for human and ecological effects.

sources (such as automobiles) (EPA, 1991a). In addition to exclusion of certain industrial sectors, not all toxic chemicals are reported to the Toxics Release Inventory. Also, companies do not need to verify the release data they submit, which results in data of unknown accuracy, although EPA is providing guidance for quality control. Finally, some companies required to report releases may not be reporting, resulting in an overall underreporting of total releases.

Despite the fact that the TRI database does not capture all chemicals, industrial sectors, or releases of concern to both OPPT and the Agency as a whole, EPCRA Section 313 explicitly provides for the expansion of TRI to cover additional chemicals and industries. As mentioned earlier, EPA recently added nearly 300 chemicals to the original reporting requirements. Moreover, with continued reporting, the quality of data reported to the Toxics Release Inventory is assumed to be improving (EPA, 1991a), and OPPT also performs quality control/ quality assurance activities. Finally, the TRI Relative Risk-based Environmental Indicators computer program allows the user to import other types of data to be used in conjunction with (or in place of) TRI data, if chemical toxicity, physicochemical properties and release quantities and locations are known.

A limitation to the interpretation of the TRI Relative Risk-based Environmental Indicators is identifying the underlying causes of changes in the Indicator values. Although the Indicator will track reductions that result from both government regulations and from voluntary industry actions, it is not possible to discern the relative magnitude of reductions attributable to a particular type of action, unless specific reductions in emissions can be attributed to particular actions.

#### **HOW INDICATOR TOXICITY WEIGHTINGS DIFFER FROM EPCRA SECTION 313 STATUTORY CRITERIA**

The TRI Relative Risk-Based Environmental Indicators utilize Toxics Release Inventory (TRI) chemical reporting data. All of the TRI chemicals included in the Indicators are listed on the TRI because they meet one or more statutory criteria regarding acute or chronic human toxicity, or environmental toxicity. The goal of the Indicators is to use data reported to the Agency to investigate the relative risk-based impacts of the releases and transfers of these chemicals on the general, non-worker population.

To do this, the Indicators must differentiate the relative toxicity of listed chemicals and rank them in a consistent manner. The ranking of each chemical reflects its toxicity only relative to other chemicals which are included in the Indicators; not to some benchmark or absolute value.

The TRI Relative Risk-Based Chronic Human Health Indicator addresses only the single, most sensitive chronic human health toxicity endpoint. Unlike the statutory criteria used for listing and delisting chemicals, the Indicator does not address the absolute chronic toxicity of chemicals on the TRI (e.g., multiple effects or the severity of effects); nor does it attempt to reflect the statutory criteria for these chemicals.

It is important that the public not confuse the use of the Indicator as a screening-level tool for investigating relative risk-based impacts related to the releases and transfers of TRI chemicals, with the very different and separate activity of listing/delisting chemicals on the TRI using statutory criteria. The toxicity weightings provided in the Indicator method cannot be used as a scoring system for evaluating listing/delisting decisions.

### **Emergency Planning and Community Right-to-Know Act Section 313 Statutory Criteria**

The Emergency Planning and Community Right-to-Know Act of 1986 (EPCRA) section 313(d)(2) sets out criteria for adding chemicals to the list of chemicals subject to reporting under EPCRA section 313(a). For a chemical (or category of chemicals) to be added to the EPCRA section 313(c) list of toxic chemicals, the Administrator must judge whether there is sufficient evidence to establish any one of the following:

Acute Human Toxicity §313(d)(2)(A) - The chemical is known to cause or can reasonably be anticipated to cause significant adverse acute human health effects at concentration levels that are reasonably likely to exist beyond facility site boundaries as a result of continuous, or frequently recurring, releases.

Chronic Human Toxicity §313(d)(2)(B) - The chemical is known to cause or can reasonably be anticipated to cause in humans—

- (i) cancer or teratogenic effects, or
- (ii) serious or irreversible—
  - (I) reproductive dysfunctions,
  - (II) neurological disorders,
  - (III) heritable genetic mutations, or
  - (IV) other chronic health effects.

Environmental Toxicity §313(d)(2)(C) - The chemical is known to cause or can reasonably be anticipated to cause, because of—

- (i) its toxicity,
- (ii) its toxicity and persistence in the environment, or
- (iii) its toxicity and tendency to bioaccumulate in the environment, significant adverse effect on the environment of sufficient seriousness, in the judgement of the Administrator, to warrant reporting under this section.

To remove a chemical from the section 313(c) list, the Administrator must determine that there is not sufficient evidence to establish any of the criteria described above as required by EPCRA section 313(d)(3).

The EPA examines all of the studies available for a chemical to decide if the chemical is capable of causing any of the adverse health effects or environmental toxicity in the criteria. Agency guidelines describe when a study shows such effects as cancer (EPA, 1986a), developmental toxicity (teratogenic effects) (EPA, 1991b), or heritable genetic mutations (EPA, 1986b). The review makes a qualitative judgment regarding the potential of each chemical to meet at least one of the criteria and the chemical is added to the list if this judgment is positive. If a chemical is on the list and it is not possible to make a positive judgment regarding any of the criteria, then the chemical can be removed. There is no correlation between the toxicity criteria and methodology used to make listing decisions under EPCRA section 313 and the methodology used to rank chemicals for the Indicators.

### **Relative Toxicity Weighting of Chemicals in the TRI Relative Risk-Based Chronic Human Health Indicator**

In order to help the Agency make decisions, comparisons can be made among chemicals once they are listed under EPCRA section 313. The TRI Chronic Human Health Indicator considers aspects of the adverse health effects (cancer and noncancer), along with exposure and population weighting factors, to permit the chemicals to be ranked relative to one another. These aspects are available in public Agency-generated databases. Uncertainty reflecting the quality and adequacy of the data is incorporated into a toxicity weighting each chemical receives. The approach is intended to differentiate the relative toxicity of these chemicals in a uniform manner, provide a clear and reproducible scoring system based upon easily accessible and publicly available information, and utilize EPA consensus opinion to the greatest extent possible.

A complete discussion of the methods used in deriving the toxicity weightings for the Indicator, as well as the chemical-specific data summaries and scores, is provided in the document, *TRI Relative Risk-Based Environmental Indicators Project: Interim Toxicity Weighting Summary Document* (EPA, 1997).

## **II. GENERAL DESCRIPTION OF THE TRI RELATIVE RISK-BASED ENVIRONMENTAL INDICATORS**

### **APPROACHES USED TO ADJUST RELEASES AND TRANSFERS IN OTHER EXISTING SCREENING SYSTEMS**

Offices within EPA and organizations outside the Agency have developed numerous systems for scoring or weighting chemicals based on potential toxicity and/or exposure. The usual purpose of such activities is to prioritize chemicals for further study or for closer regulatory scrutiny, or to target chemicals or industries for enforcement. A review of chemical scoring and ranking procedures is presented in Appendix A. These systems were reviewed (before the TRI Relative Risk-based Environmental Indicators method was developed), to learn from the successes and problems of earlier efforts.

Previous scoring systems have used a variety of methods to weight chemicals. The actual numerical weights applied to chemicals can be qualitative, ordinal, proportional or calculated, or some combination of these approaches. The relative severity of the effects posed by chemicals can also be included, as can considerations of the quality of the toxicity data and exposure estimates. Based on our review of these scoring systems, several options for an evaluation method emerged. Alternative methods, and their advantages and disadvantages, were considered by the TRI Relative Risk-based Environmental Indicators Work Group and are summarized in Appendix B. This report presents a method based on the research described in Appendices A and B and based on Work Group deliberations. While the method described in this document contains elements of the options described in Appendix B, the TRI Relative Risk-based Environmental Indicators method combines these elements in a manner that is not presented explicitly in that appendix.

## **GENERAL APPROACH USED FOR THE TRI RELATIVE RISK-BASED ENVIRONMENTAL INDICATORS**

This report describes the method for constructing the TRI Chronic Human Health Indicator and a draft method for the TRI Chronic Ecological Indicator. For both, the objective is to calculate a unitless value that reflects the relative risk-related impacts of releases and transfers of all included TRI chemicals from all reporting facilities to each environmental medium for a given year or years.

To construct Indicators that are related to risk, the reported quantity of TRI releases and transfers must be adjusted in a manner that relates to the risks associated with each media-specific release or transfer of each chemical. The risk potentially posed by a chemical release depends on the inherent toxicity of the chemical, the environmental fate and transport of the chemical in the medium to which it is released, the degree of contact between the contaminated medium and the human or ecological receptors, and the size of the exposed population. Differences in these factors influence the relative contribution each release or transfer makes to each Indicator. Transfers to off-site locations such as sewage treatment plants (POTWs) require an additional estimate of the impact of treatment technologies on the magnitude of release and are modeled based upon exposure and population parameters associated with that site.

In order to incorporate these factors into the Indicators, three main components are used to compute each Indicator. These are:

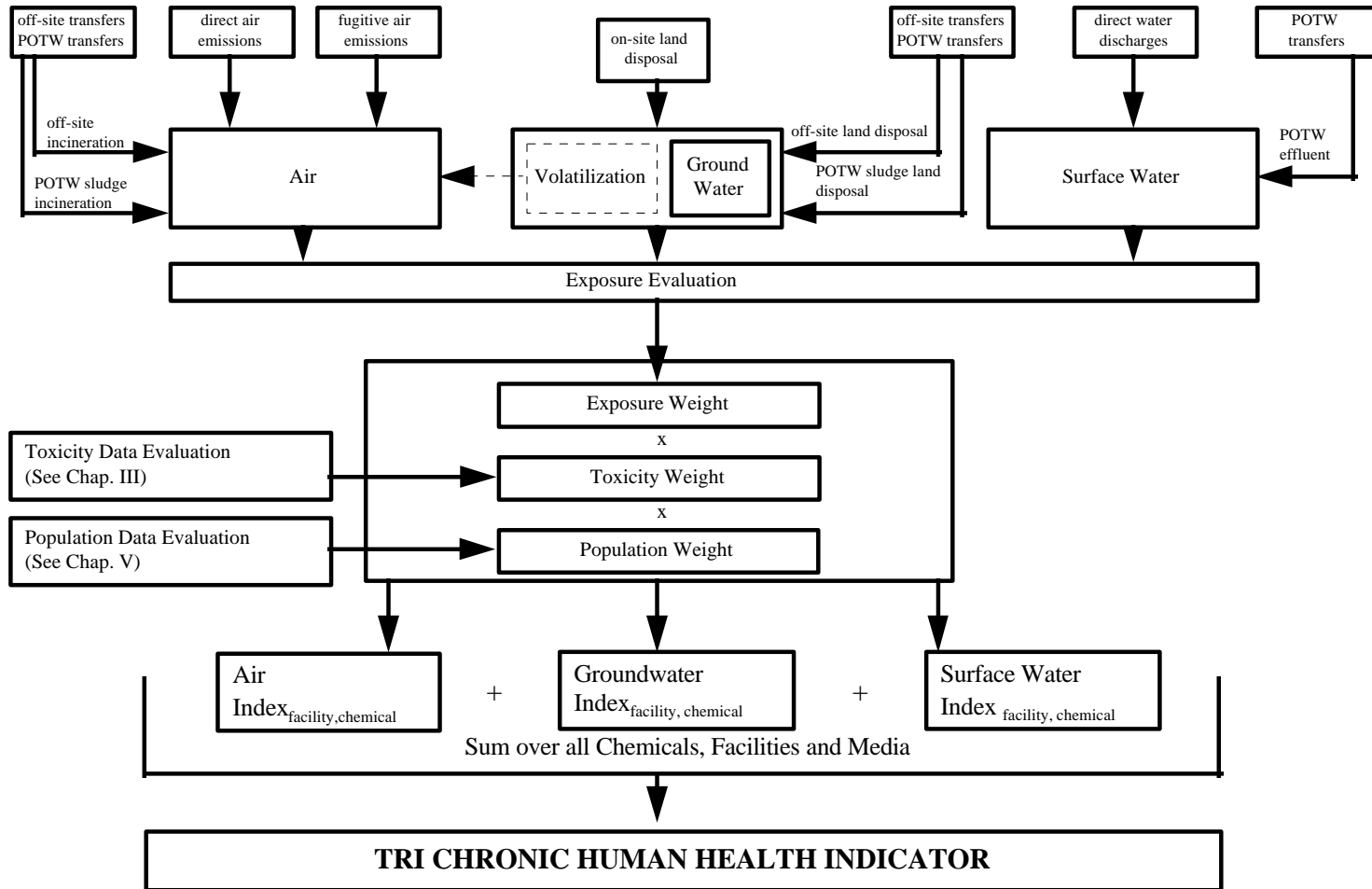
- the quantity of chemicals released or transferred,
- adjustments for chemical-specific toxicity (described in chapter III), and
- adjustments for pathway-specific and chemical-specific exposure potential (described in chapter IV).

An additional adjustment is applied to the Chronic Human Health Indicator to reflect size of the potentially exposed population<sup>2</sup> (see chapter V). This basic outline is illustrated in Exhibit 1.

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<sup>2</sup>The method focuses on general populations: individuals, particularly highly exposed individuals, are not the focus of the Chronic Human Health Indicator. Furthermore, worker exposures are not addressed. Additional Indicators based upon highly exposed or sensitive subpopulations may be developed in the future.

## EXHIBIT 1. Calculation of TRI Chronic Human Health Indicator



The TRI Chronic Human Health Indicator uses these components to perform a separate assessment for each unique combination of a chemical, facility, and release or transfer medium. Each of these releases or transfers results in a calculated “Indicator Element,” a unitless value proportional to the potential risk-based impact of each specific release or transfer. The value for the TRI Chronic Human Health Indicator is simply the sum of all the applicable Indicator Elements. Similarly, for the TRI Chronic Ecological Indicator, a separate assessment is made for each unique chemical-facility combination affecting the water medium, yielding the Ecological Indicator elements. The overall TRI Chronic Ecological Indicator is the sum of these elements. Chapter VI presents the specific equations for the calculation of each of these Indicators.

The overall Indicators are calculated for each year in the TRI data set, beginning with 1988. These values can be compared in a number of ways. For example, one of the early years of TRI reporting, 1988 for example, may be selected as the “base year” and later years’ Indicator values are compared to it. For the base year, the unitless score is scaled to 100,000 by dividing the summation of the Indicator Elements and multiplying by 100,000; subsequent years’ data are scaled by the same factor (i.e., normalized) to provide a relative comparison. This comparison allows assessment of the changes in estimated risk-related impacts of TRI releases and transfers from year to year.

Importantly, the TRI Relative Risk-based Environmental Indicators method offers unlimited combinations and views of the Indicators’ subcomponents. Each facility-chemical-media Indicator Element is retained by the computer program and thus can be evaluated by users wishing to investigate the structure of the Indicators. OPPT, other EPA Offices, Regions, States, or individuals could use these individual elements to create their own “subindicators” that examine the Indicator from alternative perspectives, such as chemicals, industries, or geographic regions (among other parameters).

It must be emphasized that the TRI Relative Risk-based Environmental Indicators method is not intended to be a quantitative risk assessment and does not calculate risk estimates. The method follows the same general paradigm often applied in quantitative assessments, but in a relative way. The TRI Relative Risk-based Environmental Indicators are by their nature only intended to reflect the direction and the general magnitude of the change in releases over time, scaled by factors (toxicity, exposure potential, and population size) that relate to potential risk. As such, an Indicator value has only relative rather than absolute meaning; it can only be used in comparisons to other Indicator values at different points in time, or in identifying the relative size of contributing factors to the overall Indicator score.

The following four chapters of this report describe the methods used for making toxicity, exposure potential and population adjustments to the emissions data, and also present the equations for calculating the overall Indicators values. Subsequent chapters discuss implementation issues related to the use of the TRI Relative Risk-based Environmental Indicators, as well as ideas for future improvements and/or additions to the set of Indicators.

Though this document presents conceptual methods for both the TRI Chronic Human Health Indicator and the TRI Chronic Ecological Indicator, the method has only been implemented for the TRI Chronic Human Health Indicator. Further method development, and further data collection and analysis, will be required for the implementation of the TRI Chronic Ecological Indicator.

### **III. METHODS FOR CALCULATING TOXICITY WEIGHTS**

#### **CHRONIC TOXICITY WEIGHTS — HUMAN**

The Section 313 criteria list several human toxicity parameters that EPA must consider when evaluating a chemical for addition to TRI, including acute toxicity, cancer or teratogenic effects, serious or irreversible reproductive dysfunctions, neurological disorders, heritable genetic mutations, or other chronic health effects, and environmental toxicity. Some chemicals have toxicity data for only one effect, while others will have evidence of effects within several of these toxicity categories. The definition of these parameters, as given in Section 313, are given in Exhibit 2. A release could be weighted based upon the number of these effects that it causes, the relative severity of the effects it causes, the potency of the chemical for one or more of these effects and the uncertainty inherent in characterizing effects.

The TRI Relative Risk-based Environmental Indicators method for developing chronic human health toxicity weights focuses on the latter two factors. It thus considers both qualitative and quantitative elements to judge the relative toxicity of chemicals. There is uncertainty inherent in determining both whether exposure to a chemical will cause an effect in humans and the potency of the chemical. Quantitative potency data must be considered in the context of a qualitative classification of the uncertainty associated with that data. In the case of noncancer effects, this classification is considered in the development of the quantitative toxicity values (e.g., Reference Dose values). However, for chemicals with carcinogenic effects, the TRI Relative Risk-based Environmental Indicators method uses existing qualitative weight-of-evidence (WOE) measures in addition to quantitative toxicity values to assign toxicity weights.

#### **Qualitative Data Used in Chronic Human Toxicity Weighting**

Risk assessors use a variety of data to evaluate the potential toxicity of a chemical to humans, including epidemiological data, data from acute and chronic animal studies, and in vitro toxicity tests. Together, these data form a body of evidence regarding the potential for toxic chemicals to cause a particular health effect in humans. The risk assessor can judge qualitatively the strengths of this body of evidence when determining the probability of the occurrence of the effect in humans. Based on this judgment, the chemical is assigned a WOE classification. Weight-of-evidence schemes can be designed to indicate whether a chemical either causes a specific health effect in

## EXHIBIT 2. Toxicity Endpoints

Endpoint	Definition
Carcinogenicity	This toxicity endpoint concerns the ability of a chemical to produce cancer in animals or humans.
Heritable Genetic and Chromosomal Mutation	Chemicals which affect this endpoint can cause at least three separate modes of failure to transmit genetic information: gain or loss of whole chromosomes (aneuploidization), rearrangement of parts of chromosomes (clastogenesis), and addition or deletion of a small number of base pairs (mutagenesis).
Developmental Toxicity	Any detrimental effect produced by exposures to developing organisms during embryonic stages of development, resulting in: prenatal or early postnatal death, structural abnormalities, altered growth, and functional deficits (reduced immunological competence, learning disorders, etc.).
Reproductive Toxicity	This endpoint concerns the development of normal reproductive capacity. Chemicals can affect gonadal function, the estrous cycle, mating behavior, conception, parturition, lactation, and weaning.
Acute Toxicity	Acute toxicity indicates the potential for a short-term exposure (typically hours or days) by inhalation, oral, or dermal routes to cause acute health effect or death.
Chronic Toxicity	Chronic toxicity indicates the potential for any adverse effects other than cancer observed in humans or animals resulting from long-term exposure (typically months or years) to a chemical.
Neurotoxicity	This endpoint concerns the central and/or peripheral nervous system. Changes to the system may be morphological (biochemical changes in the system or neurological diseases) or functional (behavioral, electrophysiological, or neurochemical effects).

general, or specifically in humans. The carcinogenicity WOE system presented in this methodology relies on categorical definitions from the EPA Guidelines for Carcinogenic Risk Assessment (EPA, 1986a, currently being revised), which are related to the potential for a chemical's carcinogenicity in humans. These Guidelines define the following six WOE categories, as shown in Exhibit 3:

**EXHIBIT 3. Weight of Evidence Categories for Carcinogenicity**

<b>Category</b>	<b>Weight of Evidence</b>
A	Sufficient evidence from epidemiological studies to support a causal relationship between exposure to the agent and cancer.
B1	Limited evidence from epidemiological studies and sufficient animal data.
B2	Sufficient evidence from animal studies but inadequate or no evidence or no data from epidemiological studies.
C	Limited evidence of carcinogenicity in animals and an absence of evidence or data in humans.
D	Inadequate human and animal evidence for carcinogenicity or no data.
E	No evidence for carcinogenicity in at least two adequate animal tests in different species or in both adequate epidemiological and animal studies, coupled with no evidence or data in epidemiological studies.

For noncancer effects, weight-of-evidence is considered qualitatively in the hazard identification step of determining a Reference Dose (RfD) (see below for discussion of RfD). The WOE evaluation for noncancer effects is different from that for carcinogenic effects. For exposure to chemicals with potential carcinogenic effects, current EPA policy assumes no threshold exposure below which cancer risk is zero; thus, determining a chemical to be a known, probable, or possible human carcinogen implies some risk associated with any exposure. Therefore the WOE determination focuses on whether the chemical may or may not cause cancer in humans. In contrast, the judgment that a chemical is a systemic toxicant is dose-dependent; the WOE evaluation focuses on the dose where chemical exposure would be relevant to humans (Dourson, 1993). The focus of the WOE evaluation, and the expression of the level of confidence in the RfD, is a judgment of the accuracy with which the dose relevant to humans has been estimated. The WOE evaluation is included qualitatively in the RfD, but does not affect its numerical calculation. Since weight of evidence has been considered in developing RfDs, the TRI Relative Risk-based Environmental Indicators method does not consider WOE separately for noncancer effects.

## Quantitative Data Used in Chronic Human Toxicity Weighting

### *Types of Data*

Quantitative data on the relative potencies of chemicals are needed for toxicity weighting. For **cancer risk assessment**, EPA has developed standard methods for predicting the incremental lifetime risk of cancer per dose of a chemical. EPA generally uses a linearized multistage model of carcinogenesis to quantitatively model the dose-response function of a potential carcinogen. The upper bound of the linear term of this model is called the  $q_1^*$ . This slope factor is a measure of cancer potency. Cancer risk can also be expressed as a unit risk factor, that is, the incremental lifetime risk of cancer per  $\text{mg}/\text{m}^3$  in air or per  $\text{mg}/\text{L}$  in water. Although the level of conservatism inherent in these slope factors and unit risk factors varies by chemical, unit risk factors and  $q_1^*$ s nonetheless are the best readily available values that allow us to compare the relative cancer potency of chemicals.

For **noncancer risks**, data on dose-response are more limited; generally, a risk assessor evaluates dose compared to a Reference Dose (RfD) or Inhalation Reference Concentration (RfC). Both the RfD and RfC are defined as “an estimate (with uncertainty spanning perhaps an order of magnitude) of a daily exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime” (EPA, 1988a; EPA, 1990g). The units of RfD are  $\text{mg}/\text{kg}\text{-day}$ , while the units of the Inhalation Reference Concentration are  $\text{mg}/\text{m}^3$ . A chemical’s reference dose or reference concentration is based on a No Observable Adverse Effect Level or Lowest Observable Adverse Effect Level, combined with appropriate uncertainty factors to account for intraspecies variability in sensitivity, interspecies extrapolation, extrapolation from LOAELs to NOAELs, and extrapolation from subchronic to chronic data. In addition, a modifying factor can be applied to reflect EPA’s best professional judgment on the quality of the entire toxicity database for the chemical. By definition, exposures below the RfD are unlikely to produce an adverse effect; above this value, an exposed individual may be at risk for the effect. Empirical evidence generally shows that as the dosage of a toxicant increases, the severity and/or incidence of effect increases (EPA, 1988a), but for a given dose above the RfD, the specific probability of an effect is not known, nor is its severity. For purposes of the TRI Relative Risk-based Environmental Indicator method, we assume that noncancer risk varies as the ratio of the estimated dose to the RfD.

### *Sources of Data*

Information regarding the human health effects data on the TRI chemicals was compiled from a number of sources. The primary source of these data was the Integrated Risk Information System (IRIS). This computerized data source includes information on EPA evaluations of chemical toxicity for both cancer and noncancer effects of chemicals. IRIS provides both background information on the studies used to develop the toxicity evaluations and the numerical toxicity values used by EPA to characterize risks from these chemicals. These values include upper-bound slope factors ( $q_1^*$ ) or inhalation unit risk values for chemicals with carcinogenic effects as well as RfDs or RfCs for chemicals with noncancer effects. Data contained in IRIS have been peer-reviewed and represent

Agency consensus. The peer-review process involves literature review and evaluation of a chemical by individual EPA program offices and intra-Agency work groups before inclusion in IRIS.

When IRIS values are not available for TRI chemicals, an alternate source of toxicity data is the Health Effects Assessment Summary Tables (HEAST). These tables are constructed for use in both the Superfund program and in the RCRA program but do not represent overall Agency consensus. However, these tables are publicly available from the Superfund program. The tables include slope factor estimates and unit risks as well as WOE categorizations for chemicals with cancer effects, and RfDs and RfCs for noncancer effects.

In cases where IRIS or HEAST do not have toxicity values and WOE classifications, we have relied on several other sources for data from which to assign weights for use in the Indicators method. Although individual literature searches for toxicological and epidemiological data for each chemical were beyond the scope of this project, data bases such as the Hazardous Substances Data Base (HSDB), as well as various EPA and ATSDR summary documents, provided succinct summaries of toxic effects and quantitative data, toxicological and epidemiological studies, and, in some cases, regulatory status data. Summaries of these data, and suggested toxicity scores based on the summaries, were provided for selected chemicals to a group of OPPT health scientists charged with reviewing toxicity data. After their review, this group then approved or disapproved the suggested scores through a disposition process. A complete discussion of the methods used in these evaluations, as well as the chemical-by-chemical data summaries and score assignments, are provided in the document *TRI Relative Risk-based Environmental Indicators Project: Interim Toxicity Weighting Summary Document* (EPA, 1997b).

### **General Format for Combining Weight-of-Evidence and Slope Factors to Assign Weights**

Several methods for deriving toxicity weights were considered during the development of the Indicator, including using low, medium, and high categories; using ordinal scores; using order of magnitude scores for categories of toxicity; or using specific numerical risk values, such as RfDs and slope factors. The merits and disadvantages of each of these methods is discussed in Appendix B.

The method chosen is applies order of magnitude weights based on categories of toxicity. The method uses different schemes to weight the toxic effects of a chemical, depending on whether the effect is carcinogenic or noncarcinogenic. For carcinogenic effects, the method uses a matrix to evaluate a chemical based on WOE and slope factor simultaneously. Rows and columns form matrix cells to which a toxicity weight is assigned. The rows of the matrix are defined by the ranges of the slope factor, while the columns of the matrix are defined by the weight-of-evidence categorization. The toxicity values are assigned to each slope factor range-WOE combination. For noncarcinogenic effects, weights are applied based on ranges of noncancer risk values alone.

Using categorical weights for toxicity has several advantages over calculating specific, unique numerical weights for chemical releases. First, unique weights would imply that we know the toxicity of the chemical with enough accuracy to distinguish among relatively small differences in these values.

In fact, there are significant uncertainties associated with the assessment of a chemical's slope factor and even weight-of-evidence. In fact, the definition of the RfD contains the expression "within an order of magnitude." Weighting a release based on broader categories of toxicity into which it falls avoids the impression of accuracy where such accuracy does not exist. Second, when general categories are used, chemicals are likely to remain in the broad toxicity category to which they are originally assigned, unless significant new and different toxicity data become available. Broad categories are also likely to be more robust as new methods for evaluating the toxicity of chemicals (such as new approaches to cancer risk assessment) develop over time. Thus, categorical weights applied to these chemicals are not likely to be revised frequently, lending stability to the Indicators over time. Finally, defining broad categories of weights allows EPA analysts to use a wide variety of qualitative and quantitative toxicity information, including consideration of chemicals that are policy priorities for the Agency, to make approximate judgments about the relative level of concern with respect to toxicity for chemicals where specific slope factors and RfD values have not yet been developed by the Agency. This more flexible approach allows more chemicals to be included in the Indicator than would be possible if specific unique numeric risk values were required for the development of toxicity weights.

Either ordinal or proportional weights could be assigned to the categories defined by the matrix cells. Ordinal weights delineate the relative toxicity rank among emissions and are useful for setting priorities. They do not, however, provide information on the magnitude of the toxicity of chemicals relative to one another. For example, an ordinal rank of 3 for chemical A and 1 for chemical B does not mean chemical A is three times worse than chemical B. Since ordinal weights do not reflect proportional differences in toxicity, the ability of the Indicator to reflect changes in health and environmental impacts could be limited if ordinal weights are used. In fact, if ordinal weights are used, it is possible that the Indicator could decrease over a period when actual risk increases. An example of this possibility is illustrated in Exhibit 4, which compares the direction of the trend illustrated by an ordinal-based indicator to the trend shown in a hypothetical quantitative risk assessment.

Unlike ordinal systems, proportional scoring systems use numerical scores that reflect the magnitude of difference between the impacts associated with chemical releases. Exhibit 5 shows how the Indicator value developed in Exhibit 4 would change if proportional rather than ordinal weights are assigned to the categories. In the TRI Relative Risk-based Environmental Indicators method, weights increase by an order of magnitude for each order of magnitude increase in toxicity and for each increase in WOE category.

#### EXHIBIT 4. Use of an Ordinal Weighting System

Assume that the following ordinal weighting system is used to calculate the TRI Chronic Human Health Indicator. This example Indicator addresses the releases of carcinogens to air:

$q_i^*$ Value	Toxicity Weight
50 or greater	6
$5 < x < 50$	5
$0.5 < x < 5$	4
$0.05 < x < 0.5$	3
$0.005 < x < 0.05$	2
less than $< 0.005$	1

Component scores for a facility, chemical, and medium are calculated by multiplying the ordinal toxicity weight (the  $q_i^*$  ranking) by the surrogate dose and by the exposed population. The result is divided by 100 to eliminate unnecessary orders of magnitude. Assume that the TRI set of chemicals and facilities consists of two chemicals and two facilities. We have the following data:

Year	Facility	Chemical	$q_i^*$ (kg-day/mg)	Population Exposed	Surrogate Dose (mg/kg-day)	Estimated Lifetime Cases = ( $q_i^* \times \text{dose} \times \text{pop.}$ )
1	1	vinyl chloride	2.3	10,000	0.006	138
1	2	benzene	0.029	1,000,000	0.006	174
2	1	vinyl chloride	2.3	10,000	0.08	1,840
2	2	benzene	0.029	1,000,000	0.003	87

The corresponding scores would be:

Year	Facility	Chemical	Toxicity Weight	Population Exposed	Surrogate Dose (mg/kg-day)	Overall Score
1	1	vinyl chloride	4	10,000	0.006	2.4
1	2	benzene	2	1,000,000	0.006	120
2	1	vinyl chloride	4	10,000	0.08	32
2	2	benzene	2	1,000,000	0.003	60

The overall TRI Chronic Human Health Indicator (i.e., the sum of the scores from the two facilities) for year one is 122, while for year two it is 92. Thus, from the Indicator, it would appear as if health risks have decreased. However, the actual number of total estimated cancer cases has increased dramatically, from roughly 310 to over 1,900.

## EXHIBIT 5. Use of a Proportional Weighting System

Assume that the following proportional weighting system is used to calculate the TRI Chronic Human Health Indicator. As in Exhibit 4, the example Indicator addresses the releases of carcinogens to air:

$q_i^*$ Value	Toxicity Weight
50 or greater	1,000,000
$5 < x < 50$	100,000
$0.5 < x < 5$	10,000
$0.05 < x < 0.5$	1,000
$0.005 < x < 0.05$	100
less than 0.005	10

Component scores for a facility, chemical, and medium are calculated by multiplying the proportional toxicity weight (the  $q_i^*$  ranking) by the surrogate dose and by the exposed population. The result is divided by 10,000 to eliminate unnecessary orders of magnitude. Assume that the example TRI set of chemicals and facilities consists of two chemicals and two facilities. We have the following data:

Year	Facility	Chemical	$q_i^*$ (kg-day/mg)	Population Exposed	Surrogate Dose (mg/kg-day)	Estimated Lifetime Cases = ( $q_i^* \times \text{dose} \times \text{pop.}$ )
1	1	vinyl chloride	2.3	10,000	0.006	138
1	2	benzene	0.029	1,000,000	0.006	174
2	1	vinyl chloride	2.3	10,000	0.08	1,840
2	2	benzene	0.029	1,000,000	0.003	87

The corresponding scores would be:

Year	Facility	Chemical	Toxicity Weight (for A/B carcinogen)	Population Exposed	Surrogate Dose (mg/kg-day)	Overall Score
1	1	vinyl chloride	10,000	10,000	0.006	6
1	2	benzene	100	1,000,000	0.006	6
2	1	vinyl chloride	10,000	10,000	0.08	80
2	2	benzene	100	1,000,000	0.003	3

Using proportional weighting, the overall TRI Chronic Human Health Indicator (the sum of the scores for the two facilities) for year one is 12, while for year two it is 83. Thus the increase in risk portrayed by the Indicator successfully reflects the trend of the increase in the estimated number of cancer cases.

## The Human Health Toxicity Weighting Schemes

The preceding discussion presented the general framework for weighting the toxicity of TRI releases. This section describes and explains the specific weighting schemes developed from this framework. Two separate toxicity weighting schemes, for carcinogenic effects and noncancer effects, are discussed (see Exhibits 6 and 7).

### *Carcinogenic Effects*

When EPA-derived values are available regarding the carcinogenicity of a chemical, the following matrix for chemicals with potential carcinogenic effects is applied:

**EXHIBIT 6. Toxicity Weighting Matrix for Carcinogenic Effects**

Range of Oral Slope Factor (risk per mg/kg-day)	Range of Inhalation Unit Risk (risk per mg/m <sup>3</sup> )	Weight of Evidence Category	
		A/B (Known/Probable)	C (Possible)
< 0.005	< 0.0014	10	1
0.005 to < 0.05	0.0014 to < 0.014	100	10
0.05 to < 0.5	0.014 to < 0.14	1000	100
0.5 to < 5	0.14 to < 1.4	10,000	1000
5 to < 50	1.4 to < 14	100,000	10,000
≥ 50	≥ 14	1,000,000	100,000

The rows of the matrix describe the ranges of slope factors used by the Indicators. The particular ranges of slope factor values selected to represent each category correspond to the ranges presented in EPA's Hazard Ranking System (HRS) (EPA, 1990b)<sup>3</sup>. The HRS is a multipathway scoring system "used to assess the threat associated with actual or potential releases of hazardous substances at sites" (EPA, 1990b). The HRS score determines whether a site will be included on the National Priorities List (NPL). Part of the HRS scoring system rates the inherent toxicity of chemicals based on measures of cancer slope factor, RfDs, and/or acute toxicity. Ranges of slope factors that differ by an order of magnitude are assigned scores that differ by an order of magnitude. The actual numerical weights assigned to the matrix cells in Exhibit 6 correspond to the scores

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<sup>3</sup>Note that only the toxicity weighting schemes (for human health and aquatic toxicity) from HRS are used. No other weighting schemes from the HRS are used in the Indicators method.

assigned in the HRS to these slope factor ranges. [Recall that slope factors are expressed as risk per unit dose in mg/kg-day.] In certain cases, ranges presented in the Indicator's matrix extend beyond those presented in the HRS because the range of slope factors for the TRI chemicals is broader than that covered by the HRS. Chemicals with slope factors smaller than a risk of 0.005 per mg/kg-day are assigned the lowest toxicity weight while those with slope factors greater than 50 are assigned the highest toxicity weight.

The columns of the matrix qualitatively classify the potential carcinogenicity of a chemical into two general categories: known/probable and possible. Weight-of-evidence categories A, B1 and B2 of the EPA Cancer Risk Assessment Guidelines are placed in the "known/probable" category. Class C is placed in the "possible" category. Categories D and E are not considered in this weighting scheme. The combination of the A and B categories represents a modification of the HRS scoring system, where A, B and C categories are each scored separately. This modification and one other (see below) were made based upon comments received from two of the 1992 peer reviewer's: Adam Finkel, Sc.D. (Resources for the Future) and John Graham, Ph.D. (Harvard Center for Risk Analysis). These reviewers felt that this may reduce the potential of a false dichotomy between the A and B categories, which would be inappropriate for quantitative potency adjustments of this type; and because it has the advantage of stabilizing the Indicator against changes induced by chemicals shuttling between the A and B categories.<sup>4</sup>

The cells in the first WOE Category column of the matrix (that is, the column that corresponds to the "known/probable" WOE category) were assigned the weights based on the HRS values. Weights in the other column (i.e., the "possible" WOE category) were assigned by dividing the weights in the first column by a factor of 10, because evidence that they cause cancer in humans is less certain. The choice of applying a factor of 10 is on the advice of peer review; an order of magnitude is an arbitrary uncertainty factor.

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<sup>4</sup>This scoring system also differs from HRS in that it does not assign a toxicity weight of 10,000 to asbestos and to lead.

## *Noncancer Effects*

When RfD or RfC values are available, the following table is used to assign toxicity weights to chemicals associated with noncancer endpoints:

**EXHIBIT 7. Toxicity Weights for Noncancer Effects**

RfD Range (mg/kg-day)	RfC Range (mg/m <sup>3</sup> )	Assigned Weight
$0.5 \leq \text{RfD}$	$1.8 \leq \text{RfC}$	1
$0.05 \leq \text{RfD} < 0.5$	$0.18 \leq \text{RfC} < 1.8$	10
$0.005 \leq \text{RfD} < 0.05$	$0.018 \leq \text{RfC} < 0.18$	100
$0.0005 \leq \text{RfD} < 0.005$	$0.0018 \leq \text{RfC} < 0.018$	1,000
$0.00005 \leq \text{RfD} < 0.0005$	$0.00018 \leq \text{RfC} < 0.0018$	10,000
$\text{RfD} < 0.00005$	$\text{RfC} < 0.00018$	100,000

This weighting system is taken directly from the HRS, with the exception of the highest weighting category. The weight assigned to this category is logically consistent with the HRS scoring system: RfDs and interim RfDs less than 0.00005 are assigned a weight that is an order of magnitude greater than RfDs between 0.00005 and 0.0005. Weight-of-evidence is considered only qualitatively since it is taken into account in the development of the RfD.

### **Selecting the Final Chronic Human Health Toxicity Weight for a Chemical**

Chemicals can cause several types of toxic effects. The TRI Chronic Human Health Indicator weights a chemical based on the single most sensitive adverse effect for a given exposure pathway (either oral or inhalation). If a chemical exhibits both carcinogenic and noncarcinogenic effects, the higher of the associated cancer and noncancer weights is assigned as the final weight for the chemical for the given pathway.

The approach of weighting based on the most sensitive adverse effect does not consider differences in the severity of the effects posed by the chemicals. For example, the liver toxicity is weighted in the same way that neurotoxicity is weighted. Also, chemicals with a broad range of adverse health effects are weighted the same as a chemical causing only one effect. Applying additional weights reflecting severity of effect across categories of toxic endpoints would require a subjective evaluation of the relative severity of the health effects. In addition, a chemical may appear to demonstrate just one adverse effect only because there are no data on other effects; thus, applying

a weight based on the number of endpoints may undervalue some poorly studied but still risky chemicals. For these reasons, the options for applying additional weights based on number and severity of endpoints were rejected.<sup>5</sup>

Although choosing the most sensitive endpoint to weight a given chemical does not explicitly consider severity of cancer and noncancer effects within each of these groups, the method of separately weighting carcinogenic and noncarcinogenic effects cannot avoid equating toxicity values between these groups. For example, the weighting scheme equates a  $q_1^*$  value of 0.1 risk per mg/kg-day for a known/probable carcinogen with an RfD of 0.001 mg/kg-day, since both are assigned a weight of 1000 (as is done in the HRS scoring system). If one were to use this weighting scheme to evaluate actual doses, this weighting would imply that a cancer risk of  $1 \times 10^{-4}$  would be equated to a noncancer risk at the RfD.<sup>6</sup>

Inhalation and oral toxicity weights are developed separately. If values are available for each route, then separate values are assigned to each route. If data are available for only one route, the same toxicity weight generally is applied for both routes. In rare instances, toxicity studies are available to show that a given chemical causes no effects via one route; in these instances, we assign the toxicity weight only to the route that results in effects. Although assigning the same weight to both routes is not an ideal method, it is sufficient for the TRI Relative Risk-based Environmental Indicators method, which relies on order-of-magnitude weights. The alternative would be to leave out chemicals with no toxicity data for a given exposure route; this would be undesirable, since one aim of the Indicators method is to include as many chemicals as possible.

Scoring for all of the current TRI Indicators chemicals is discussed in the Toxicity Weighting Summary Document (EPA, 1997) and is summarized in Appendix C of this document.

## **CHRONIC TOXICITY WEIGHTS — ECOLOGICAL**

For ecological effects, the TRI Ecological Chronic Effects Indicator focuses on *aquatic* life impacts only. Very little data are available for most chemicals on effects to terrestrial or avian species; we assume the Chronic Human Health Indicator will provide some predictor of these.

Aquatic toxicity weighting differs from chronic human health toxicity weighting in two important respects. First, WOE is not considered a factor in the weighting scheme, since direct evidence of chemical toxicity is available from tests on aquatic species. Second, the aquatic toxicity weighting scheme simultaneously considers toxicity and bioaccumulation potential. Both of these measures are considered important when evaluating impacts on aquatic ecosystems.

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<sup>5</sup>Although we do not apply subjective weights based on number and severity of effects, the assignment of weights based on the most sensitive effect is a subjective decision in itself.

<sup>6</sup>At a dose of 0.001 mg/kg-day, a chemical with a  $q_1^*$  of 0.1 (kg-day/mg) would yield a risk of  $1 \times 10^{-4}$ .

## **Data Used in Chronic Aquatic Toxicity Weighting**

The preferred numerical aquatic toxicity data to use for weighting are the Chronic Ambient Water Quality Criteria (AWQC), developed by the Office of Water. However, Acute AWQC may be used if chronic values are not available. If neither of these values are available, the lowest LC<sub>50</sub> (the chemical concentration in water at which 50 percent of test organisms die) may be used for scoring.

The preferred measure of bioaccumulation potential is the bioconcentration factor (BCF). The BCF values are derived from laboratory tests that compare the contaminant concentration in the environmental medium (i.e., water) to the concentration in the tissues of a test organism (usually fish). Several researchers have found that for organic contaminants, the BCF can be approximated as a function of the log of the octanol water partition coefficient (log K<sub>ow</sub>). The K<sub>ow</sub> is a physicochemical property that describes the partitioning of organic chemicals between an organic solvent (octanol) and water. If BCF values are not available, the K<sub>ow</sub> can be used instead for scoring organic chemicals. Finally, when neither of these measures are available, the bioaccumulation potential can also be approximated by the water solubility of the chemical. Generally, the less soluble a chemical, the greater its potential for bioaccumulation. Values for all of these measures of bioaccumulation potential are available from a variety of sources, including the AQUIRE database, as well as a number of EPA Office of Water references, the Environmental Effects Division chemical properties data base and standard chemical reference books.

## **The Aquatic Toxicity Weighting Matrices**

The aquatic toxicity weight assigned to a chemical is a function of both its aquatic toxicity values and bioaccumulation potential values (see Exhibits 8 and 9). Separate weights are assigned based on each of these measures; the chemical's final toxicity weight is obtained by multiplying these individual weights (giving toxicity weights ranging from 0.5 to 500,000,000).

The individual weights assigned based on the measures of bioaccumulation potential are the following:

#### EXHIBIT 8. Bioaccumulation Weights

Water Solubility (mg/l)	Log K <sub>ow</sub>	BCF (L/kg)	Weight
> 1,500	<0.8	<1	0.5
-	0.8-<2	1-<10	5
-	2-<3.2	10-<100	50
>500-1,500	3.2-<4.5	100-<1,000	500
25-500	4.5-<5.5	1,000-<10,000	5,000
<25	5.5-<6.0	≥10,000	50,000

Note: If BCF values are available, they should be used; If not, log of the octanol water partition coefficient (log K<sub>ow</sub>) can be used for organic contaminants. When neither of these measures can be used, the bioaccumulation potential can also be approximated by the water solubility of the chemical. Note that K<sub>ow</sub> is not used for scoring if its value exceeds 6.0.

Individual weights based on aquatic toxicity measures are the following:

#### EXHIBIT 9. Aquatic Toxicity Weights

LC <sub>50</sub> (µg/l)	Acute AWQC (µg/l)	Chronic AWQC (µg/l)	Weight
>1,000	>100,000	>1,000	1
100-1,000	10,000-100,000	100-1,000	10
10-100	1,000-10,000	10-100	100
1-10	100-1,000	1-10	1,000
<1	<100	<1	10,000

Note: The preferred numerical aquatic toxicity data to use for weighting are the Chronic Ambient Water Quality Criteria (AWQC). Acute AWQC may be used if chronic values are not available. If neither of these values are available, the lowest LC<sub>50</sub> may be used for scoring. As shown in the table, HRS does not assign scores of 5 or 50 based on water solubility.

As with the chronic human health toxicity weighting, the quantitative measures used to represent chronic aquatic toxicity, the value ranges used to define the categories of toxicity, and the numerical weights assigned to each category were taken from the Hazard Ranking System.

Exhibit 10 presents the combined toxicity weighting system for aquatic toxicity. The rows of the matrix are defined by the bioaccumulation potential categories and the columns of the matrix are defined by the aquatic toxicity categories. The cells of the matrix are the product of the chemical's bioaccumulation potential and aquatic toxicity weights. We take the product of these values (rather than the sum or the average) because both contribute multiplicatively to the overall impact. For instance, a chemical with a toxicity weight of 10 and a bioaccumulation potential of 10 is considered to be 10 times worse than a chemical with toxicity weight of 10 and bioaccumulation potential of 1, since the potential exposure through the food chain is 10 times higher for the chemical with bioaccumulation potential of 10 versus the chemical with a bioaccumulation potential of 1.

#### **IV. METHODS FOR ADJUSTING RELEASES AND TRANSFERS FOR CHRONIC EXPOSURE POTENTIAL**

##### **EVALUATING CHRONIC HUMAN EXPOSURE POTENTIAL — GENERAL DESCRIPTION**

As with toxicity weighting, both qualitative and quantitative elements are considered when weighting chronic exposure potential. Quantitatively, release data are combined with generic exposure models to derive a “surrogate” dose level to characterize exposure potential on an exposure pathway-specific basis. Qualitatively, a level of uncertainty associated with the surrogate measures of exposure potential is assigned to each exposure pathway. The uncertainty estimates are then used to adjust the surrogate doses to derive the final exposure potential adjustment factor.

##### **Quantitative Data Used in Evaluating Chronic Human Exposure Potential**

The TRI release and transfer data are the initial source of quantitative data on potential chronic human exposure. However, the EPA has an open revision policy that allows TRI reporting facilities to submit changes and corrections to their TRI data at any time. To avoid the effects of these fluctuations on Indicator values, the TRI Indicators model extracts release and transfer data during the two week period each year when EPA Headquarters “freezes” the data, that is, when no changes are allowed.

To adjust releases and transfers to reflect exposure potential, several existing scoring systems take the approach of ordinal ranking the volume of each release by some physical measure of the chemical's ability to move through the environmental medium into which it is released. However, because the exposure potential rankings would have different physical meanings for different pathways, comparisons among different media would be difficult, and weighted releases from different pathways could not be added to obtain a single indicator value.

### EXHIBIT 10. Aquatic Toxicity Matrix

BIOACCUMULATION(a)			AQUATIC TOXICITY CATEGORY (µg/l)(b)					
Water Solubility (mg/l)	Log K <sub>ow</sub>	BCF (l/kg)	>1000	100-1000	10-100	1-10	<1	LC50
			>1000,000	10,000-100,000	1000-10,000	100-1000	<100	Acute AWQC
			>1000	100-1000	10-100	1-10	<1	Chronic AWQC
>1500	<0.8	<1	0.5	5	50	500	5000	
	0.8-2	1-10	5	50	500	5000	50,000	
	2-3.2	10-100	50	500	5000	50,000	500,000	
>500 to 1500	3.2-4.5	100-1000	500	5000	50,000	500,000	5,000,000	
25 to 500	4.5-5.5	1000-10,000	5000	50,000	500,000	5,000,000	50,000,000	
<25	5.5-6.0	>10,000	50,000	500,000	5,000,000	50,000,000	500,000,000	

Notes:

(a) If BCF values are available, they should be used; If not, log of the octanol water partition coefficient (log K<sub>ow</sub>) can be used for organic contaminants. When neither of these measures can be used, the bioaccumulation potential can also be approximated by the water solubility of the chemical. Note that K<sub>ow</sub> is not used for scoring if its value exceeds 6.0.

(b) The preferred numerical aquatic toxicity data to use for weighting are the Chronic Ambient Water Quality Criteria (AWQC). Acute AWQC may be used if chronic values are not available. If neither of these values are available, the lowest LC<sub>50</sub> may be used for scoring. As shown in the table, HRS does not assign scores of 5 or 50 based on water solubility.

In this methodology, comparisons across media can be made because a common quantitative exposure measure for each medium is derived: an estimate of “surrogate dose” — a measure related to the amount of chemical contacted by an individual per kg body weight per day. Limited facility-specific data and the use of generic models (described below) prevent the calculation of an actual dose.

To estimate the magnitude of exposure potential from TRI releases, a separate exposure evaluation is conducted for each environmental medium to which chemicals are emitted. The ideal derivation of a dose would involve a site-specific exposure assessment for each release medium and for each exposure pathway. However, such an effort is well beyond the scope of this project and well beyond the intended use of the TRI data. These data are frequently estimates of emissions, not precise measured values. Notably, they are not estimates of environmental concentrations that result from the emissions from the plant. Furthermore, reporting of extensive site-specific information relevant for exposure modeling is not part of a TRI data submission. For example, EPA Form R (Toxic Release Inventory Reporting Form) does not require submission of data on groundwater flow, soil conditions, and other factors that affect groundwater contamination from land releases. It is not the intent of this project to gather additional data or measurements that would be needed to perform these calculations. The need to accurately reflect exposure characteristics in the Chronic Human Health Indicator must be balanced by the need for a simple and understandable Indicator that is easily communicated to the public and that is based on currently available data. Therefore, in this methodology, the exposure evaluations combine data on media-specific emission volumes, physicochemical properties and, where available, site characteristics with site-specific or generic exposure models to determine an estimate of the ambient concentration of contaminant in the medium into which the chemical is released. (Again, the use of submitter-estimated TRI emission data and generic models with many default assumptions make this only a surrogate related to actual environmental concentration). For the Chronic Human Health Indicator, the ambient media concentrations are then combined with standard human exposure assumptions to estimate the magnitude of the surrogate dose. The physicochemical property data used for the exposure potential evaluation is found in Appendix D.

It must be emphasized that while this methodology uses the EPA exposure assessment paradigm to evaluate exposure potential, the results should not be construed as an actual absolute numerical estimate of dose resulting from TRI releases. Instead, the purpose is to obtain an order of magnitude estimate of surrogate dose resulting from release of TRI chemicals *relative to the surrogate dose resulting from other releases included in the Indicator*, so that these releases can be weighted appropriately in the Indicator.

Another limitation to note is that products of decay are not modeled. Exclusion of these decay products from the Indicators may underestimate or overestimate the risk impact of releases, since the decay product may be more or less toxic than the parent compound.

The exposure evaluation methods used for each type of release are specific to that type of release and depend on the models and data available to evaluate that pathway. In some cases, models will be combined with some site-specific data to estimate exposure; in other cases, generic reasonable worst-case models may be used in the absence of any site-specific data. (Specific pathway calculations are discussed below.)

### **Qualitative Data Used in Evaluating Chronic Human Exposure Potential**

Consideration of uncertainty in the exposure evaluation is necessary for making comparisons across pathways, since the exposure evaluation methods for various pathways differ significantly in their possible level of refinement. For the purposes of calculating surrogate doses, the following uncertainty categories have been defined for use in this methodology (Exhibit 11):

**EXHIBIT 11. Uncertainty Categories for Evaluating Human Exposure Potential**

<b>Category</b>	<b>Explanation</b>	<b>Adjustment Factor</b>
A	Combines modeling with some generic and some reasonable site-specific data to generate exposure estimates.	1
B	Combines modeling with some generic and some site-specific data, but identification of appropriate site-specific data subject to error and will often be filled in with generic assumptions.	5
C	Extrapolates generic exposure estimates from actual data from other sites to exposure at TRI sites (e.g., groundwater modeling).	10

The categories are defined so that surrogate dose estimates in a lower category are more likely to overestimate exposure when compared to the next higher category. In general, surrogate dose estimates are placed in lower categories when they are developed using generic models that require many assumptions and extrapolations. These assumptions and extrapolations tend to be conservative, so that more generic modeling tends to yield overestimates of exposure. The initial surrogate dose estimate is reduced by a factor of 5 if assigned to category B, and by an order of magnitude if assigned to category C.

## **PATHWAY-SPECIFIC METHODS TO EVALUATE CHRONIC HUMAN EXPOSURE POTENTIAL**

This section describes the algorithms for modeling exposure for each of the following exposure pathways: (1) stack and fugitive air releases, (2) direct surface water releases, (3) on-site land releases, (4) releases to POTWs, and (5) off-site transfers. An overview of the pathways and methodologies used for each pathway is presented in Exhibit 12.

The following discussions of exposure modeling frequently mention concentration and surrogate dose. This is not meant to imply that the risk assessment process can be supplanted nor that cases can be accurately calculated. These terms are referred to only in the abstract. The exposure algorithms are simple ways to gauge relative risks from releases to different media in a congruent, defensible way. In some cases, the modeling will be purposely simple, given our lack of site-specific data. The differences in the level of refinement of exposure modeling are addressed by using the uncertainty weighting scheme discussed above.

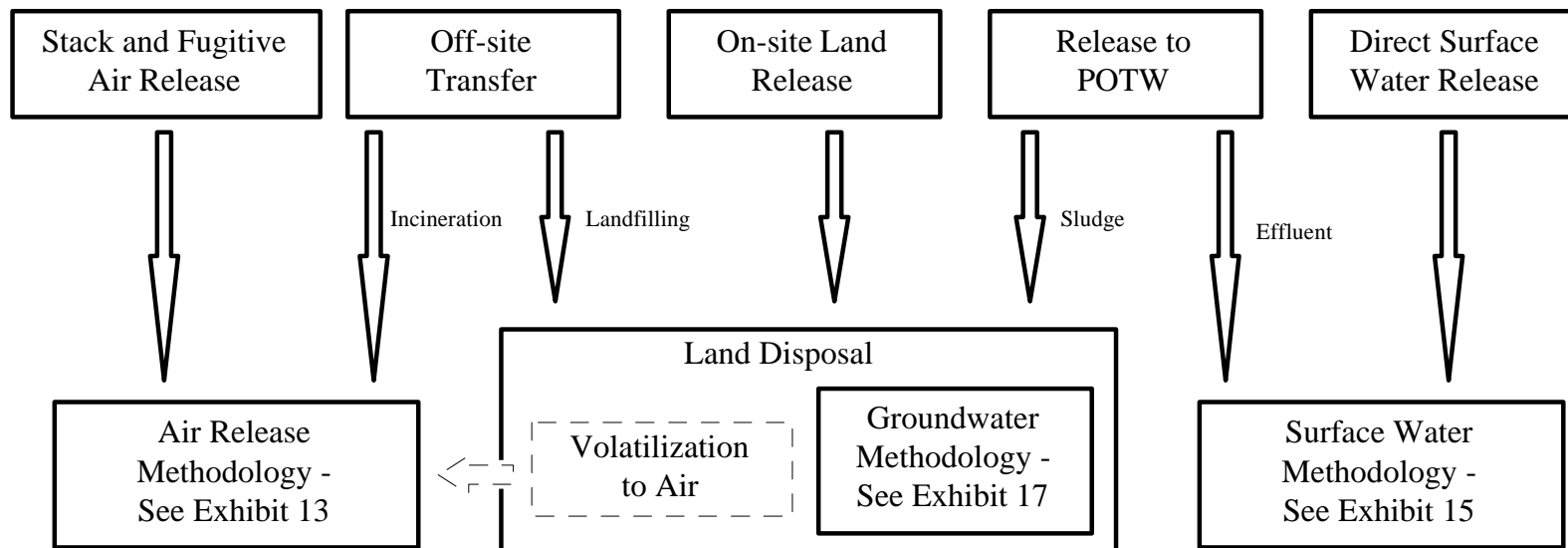
### **GIS Basis Common to All Pathways**

The algorithms for calculating surrogate doses rely on the ability to locate facilities geographically (including those to which off-site transfer is made) and to associate their locations with their demographic and physical characteristics. To accomplish this, the computer algorithm describes the U.S. as a 1 km-by-1 km grid system. For each cell in the grid, the computer assigns a location “address” based on latitude and longitude. It then assigns information on the demographics and physical characteristics of that cell to that address. (Physical characteristics include: wind speed and direction, the occurrence of a water body in the cell, and the flow rate of such a water body). When a facility is located on the grid, the associated data for that location are then automatically available for use in the modeling.

### **Stack and Fugitive Air Releases**

Ideally, reported stack and fugitive air releases from the TRI database would be modeled using site-specific data (such as stack height or source area). Because TRI does not contain such facility-specific information, default values are used to model TRI facilities using established EPA air dispersion models.

## EXHIBIT 12. Overview of Exposure Pathways



This method uses an algorithm based on the Industrial Source Complex Long Term (ISCLT) model developed by the Office of Air Quality Planning and Standards (OAQPS). ISCLT is a steady-state Gaussian plume model used to estimate long-term pollutant concentrations downwind of a source. The concentration is a function of site-specific parameters (stack height, stack gas velocity) and chemical-specific air decay rates. To use the model, the facilities are first located on the grid using their latitude and longitude coordinates. Next, their emission rates in pounds per year are directly converted to grams per second by the following equation:

$$Q = \frac{453.6 \ q}{31,536,000}$$

where:

Q	=	pollutant emission rate (g/sec),
q	=	pollutant emission rate (lb/yr),
453.6	=	constant to convert (lb) to (g), and
31,536,000	=	constant to convert (yr) to (sec).

These emissions rates are then used in the following equation that determines the concentration at a distance  $r$  greater than 1 meter away from a point source:<sup>7</sup>

$$C_{air,r_{ijk}} = \frac{K}{\sqrt{2\pi} \ r \theta} \cdot \frac{Q \ f_{ijk} \ S \ V \ D}{u_{ijk} \sigma_z}$$

where:

$C_{air}$	=	concentration at distance $r$ ( $\mu\text{g}/\text{m}^3$ ),
Q	=	pollutant emission rate (g/sec),
f	=	frequency of occurrence of wind speed and direction (dimensionless),
r	=	radial distance from point source (m),
$\theta$	=	sector width (radians),
S	=	smoothing function used to smooth discontinuities at sector boundaries (dimensionless),
u	=	mean wind speed (m/sec),
$\sigma_z$	=	standard deviation of vertical concentration distribution (m),
V	=	vertical term (dimensionless),
D	=	term for pollutant-specific decay in air, where $D=e^{r^*K_{air}/u*3600}$ , $K_{air}$ =decay rate in air ( $\text{hr}^{-1}$ ) and 3600=constant to convert (hr) to (sec), and
K	=	$10^6$ , constant to convert (g) to ( $\mu\text{g}$ )

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<sup>7</sup>This equation is from EPA (1992). The equation is for a specific wind speed, direction, and category ( $ijk$ ). Each facility has several combinations of these that must be added to arrive at a total concentration at that point. The equation for area sources is similar.

For each facility in the TRI data set, a stack height of 10 meters<sup>8</sup> is assumed to be located at the latitude and longitude of the source.

Based on the ISCLT equations, concentrations are calculated at each of the 441 cells (21 km x 21 km total area, or 10 kilometers in each direction) nearest to the facility. The concentrations are combined with standard assumptions regarding inhalation rate and human body weight to arrive at a surrogate dosage:

$$DOSE_{air} = \frac{C_{air, avg} \cdot I_{air}}{BW} \cdot \frac{1}{1000}$$

where:

$DOSE_{air}$	=	surrogate dose of contaminant from air (mg/kg-day),
$C_{air}$	=	air concentration in cell ( $\mu\text{g}/\text{m}^3$ ),
$I_{air}$	=	inhalation rate ( $\text{m}^3/\text{day}$ ),
$BW$	=	human body weight (kg), <sup>9</sup> and
1000	=	constant to convert ( $\mu\text{g}$ ) to (mg).

These surrogate doses are then multiplied by the toxicity weight for the chemical and by the population in the cell to arrive at an Indicator sub-element for each cell. If the total population in the 441 surrounding cells is less than 1000 persons, then the number of persons in the cells is adjusted such that the total population surrounding a facility is at least 1000. This is done to avoid under-weighting rural communities. The overall indicator element for the chemical and facility is determined by adding the sub-elements for all 441 cells. Exhibit 13 graphically describes the air modeling portion of the Chronic Human Health Indicator, and Exhibit 14 lists the default parameters for the air model.

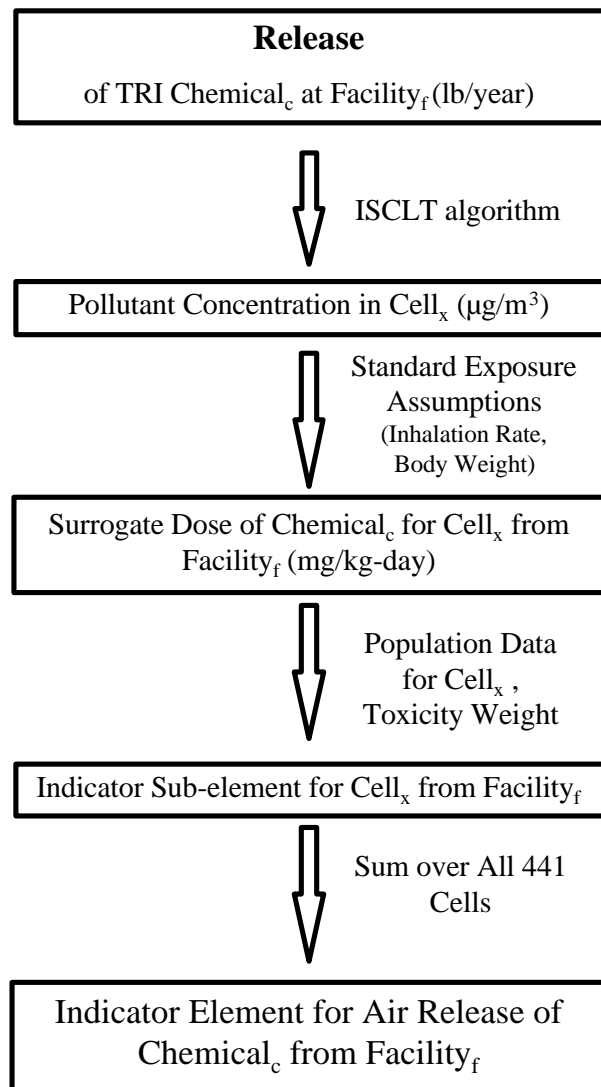
For the air release pathway, a combination of generic inputs and reasonable site-specific data (e.g., wind speed) are used. Therefore, we use uncertainty category A to classify the air exposure potential.

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<sup>8</sup>Additional information is currently being collected on industry-specific stack heights; if possible, this information will be incorporated into the model.

<sup>9</sup>This method uses an average adult body weight (70 kg). For certain health endpoints (e.g., female reproductive effects), a different body weight value may be more appropriate (e.g., average adult female body weight). However, for simplicity, the method uses the average value for all endpoints.

**EXHIBIT 13. Calculation of Surrogate Dose and Indicator Element from Stack and Fugitive Air Releases**



### EXHIBIT 14. Air Modeling Parameters

Parameter	Value	Source/Comment
Stack height	10 m	EPA (1992)
Exit velocity	0.01 m/s	EPA (1992)
Stack diameter	1 m	EPA (1992)
Exit gas temperature	293 K	EPA (1992)
Area source size	10 m <sup>2</sup>	EPA (1992)
Area source height	3 m	EPA (1992)
Decay rate	varies by pollutant	
Body weight	70 kg	EPA Exposure Factors Handbook (EPA, 1990a); value is for adults; lifetime age-weighted average (male and female combined) is about 62 kg
Pollution emission rate	site-specific	TRIS (lbs/yr)
Frequency of wind speed and direction	site-specific	STAR
Sector width	0.393 radians, or 22.5°	360° divided by 16 wind directions
Wind speed	site-specific	STAR (m/s)
Smoothing function	calculated	
Vertical term	calculated	
Population-weighted average air conc.	calculated	mg/kg-day
Inhalation rate	20 m <sup>3</sup> /day	EPA Exposure Factors Handbook (EPA, 1990a)

## Direct Surface Water Releases

As with the air pathway, the first step in assessing surface water discharges is to locate the discharging facility on the grid. Facilities are matched to a waterbody within 6 kilometers based on latitude and longitude. In the future, this match will be achieved using the NPDES (National Pollutant Discharge Elimination System) numbers provided in TRI reporting. Direct surface water discharges are assessed using a simple first-order decay equation along with water volume and velocity estimates to calculate concentrations resulting from contaminant releases at a distance  $x$  at time  $t$ . The pollutant-specific decay coefficient may be due to either abiotic hydrolysis or microbial biodegradation; on occasion, it may be due to photooxidation. The general form of the equation is as follows:

$$C_x = C_0 e^{-k_{\text{water}} t}$$

where:

$C_x$	=	concentration at distance $x$ meters (mg/L) (up to 200 kilometers from release point),
$C_0$	=	initial concentration (mg/L), which equals chemical release (mg/day) divided by water flow volume (L/day),
$k_{\text{water}}$	=	decay coefficient ( $\text{sec}^{-1}$ ),
$t$	=	time at which $C_x$ occurs (sec), which equals $x/u$ , and
$u$	=	water velocity (m/sec).

This methodology considers two chronic human health exposure pathways from surface water releases. First, exposures from drinking water are calculated. As the pollutant passes through the stream network, concentrations at public drinking water intakes are noted. The population served at each intake is assumed to be the population exposed to that concentration. If a cell contains no drinking water intake, the exposed population is zero. The water concentration in reaches with intakes is combined with standard exposure parameters to yield the following surrogate dosage:

$$DOSE_{dw} = \frac{C_{\text{water, avg}} \cdot I_{\text{water}}}{BW}$$

where:

$DOSE_{dw}$	=	surrogate dose of contaminant in drinking water (mg/kg-day),
$C_{\text{water, avg}}$	=	population-weighted average water concentration (mg/L),
$I_{\text{water}}$	=	drinking water ingestion rate (L/day), and
$BW$	=	human body weight (kg).

The Indicator sub-element for individual reaches for the drinking water pathway is calculated using the surrogate dose in the reach, drinking water population in that reach, and the toxicity weight of the chemical. For the drinking water pathway, we use uncertainty category B for exposure potential weighting for several reasons. First, the calculation of water concentrations does not consider partitioning of the chemical between the water column and suspended solids, settling of the suspended solids, volatilization of the chemical, or other processes that may affect the fate and transport of contaminants along a surface water body. Furthermore, there is no consideration of the removal of contaminants during treatment of drinking water at the utility.<sup>10</sup> All of these factors would tend to inflate the exposure potential evaluation.

A second potential exposure pathway is from consumption of contaminated fish. Each segment of the affected water body may contain contaminated fish which could be caught and eaten by recreational fishers. As described above, the program tracks the concentration of the chemical as it travels down the waterway; in each U.S.G.S.-defined stream reach, the concentration in fish is derived by the following equation:

$$C_{fish,reach} = C_{water,reach} \cdot BCF$$

where:

$$\begin{array}{ll} C_{fish, reach} & = \text{concentration in fish in the specified stream reach}^{11}, \text{ (mg/kg),} \\ C_{water, reach} & = \text{average water concentration in the specified stream reach (mg/L),} \\ & \text{and} \\ BCF & = \text{bioconcentration factor for chemical (L/kg).} \end{array}$$

Next, the fish concentration value is combined with standard exposure assumptions regarding fish consumption rates to determine the surrogate dose from this pathway:

$$DOSE_{fc} = \frac{C_{fish,reach} \cdot I_{fish}}{BW}$$

where:

$$\begin{array}{ll} DOSE_{fc} & = \text{surrogate dose of contaminant (mg/kg-day),} \\ C_{fish} & = \text{fish tissue concentration (mg/kg),} \\ I_{fish} & = \text{fish ingestion rate (kg/day), and} \\ BW & = \text{human body weight (kg).} \end{array}$$

Because specific data on people fishing in a reach are not available, the exposed population is modeled as a percentage of the drinking water population. We derived state-specific

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<sup>10</sup>Removal of contaminants during treatment could be incorporated into the analysis if data are available.

<sup>11</sup>A stream reach is defined by the U.S.G.S. as the stretch of water between an upstream confluence and the next downstream confluence. There is no constant length attributed to reach segments.

fractions of persons who eat fish from state-specific fishing rates found in the U.S. Fish and Wildlife Service's *1991 National Survey of Fishing, Hunting, and Wildlife Associated Recreation* (U.S. DOI, FWS, 1993). This estimate of exposed population, combined with the calculated surrogate dose and the toxicity weight of the chemical, gives an Indicator sub-element for fish consumption for each reach.

The total Indicator Element for surface water releases of a chemical from a facility is calculated by adding the drinking water sub-element and the fish consumption sub-element for each reach and summing over all reaches.

Exhibit 15 shows the recommended surface water approach for the Chronic Human Health Indicator, and Exhibit 16 lists model parameters for surface water modeling.

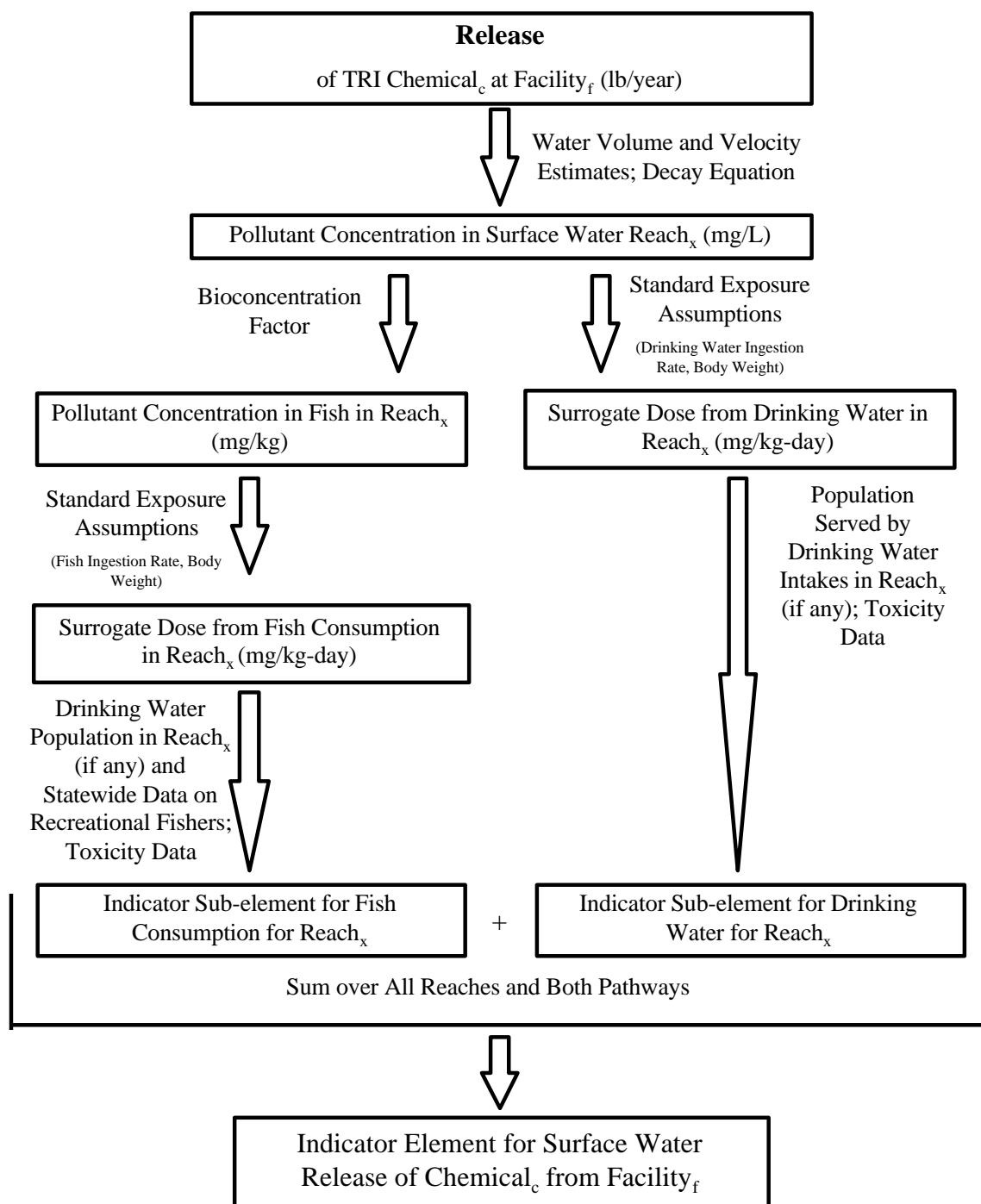
For the fish consumption exposure pathway, the method uses uncertainty category C for exposure potential for several reasons. First, as with the drinking water pathway, the estimated water concentrations are probably an overestimate because the method does not consider all fate and transport processes in surface water that affect concentrations. Second, fish tissue concentrations are dependent on the type of species, particularly its lipid content and its position in the food chain. Finally, the actual probability of recreational fishing in the particular stream reach being modeled is unknown, as is the actual quantity of fish consumed from that particular reach.

## **On-site Land Releases**

On-site land releases include releases to landfills, surface impoundments, land treatment units and underground injection. This section describes methods to evaluate exposure from these releases, except for underground injection. Under well-managed conditions, underground injection facilities are designed to pose minimal risks to human health or the environment. However, certain conditions can lead to the failure of these facilities and the release of chemicals to the environment. An exposure analysis for these releases would have to include an evaluation of the likelihood of the failure as well as a sophisticated hydrogeological evaluation of the exposure impacts of such a failure. Such an evaluation is beyond the scope of this method; at present, only the pounds of releases and transfers to underground injection releases are tracked in the computer algorithm of the Indicator. Considerations for other approaches to including underground injection in the Indicator are discussed in Appendix E.

Facilities releasing chemicals to land are located on the grid using latitude and longitude. For these releases, two major exposure pathways are considered for on-site land releases: chemicals may volatilize to air or leach to groundwater. Volatilization of chemicals from on-site landfills is reported to TRI under the fugitive emission estimate for the facility and does not have to be modeled (in contrast with volatile emissions from off-site landfills). Volatilization is thus handled as a direct air release for on-site land releases.

# **EXHIBIT 15. Calculation of Surrogate Dose and Indicator Element from Surface Water Release**



### EXHIBIT 16. Surface Water Modeling Parameters

Parameter	Value	Source/Comment
Decay rate	varies by pollutant	
Dilution rate	site-specific	REACH (EPA, 1987)
Water volume and velocity	site-specific	REACH (EPA, 1987)
Population-weighted average water concentration	calculated	mg/L
Drinking water ingestion rate	2 liters	EPA Exposure Factors Handbook (EPA, 1990a)
Body weight	70 kg	EPA Exposure Factors Handbook (EPA, 1990a); value is for adults; lifetime age-weighted average (male and female combined) is about 62 kg
Average chemical concentration in stream	calculated	mg/L
Bioconcentration factor	varies by pollutant	L/kg
Fish tissue concentration	calculated	mg/kg
Fish ingestion rate	0.0065 kg/day	Exposure Factors Handbook (EPA, 1990a)

Groundwater contamination is also a concern for land releases. However, the modeling of groundwater releases depends on the regulatory status of the unit in which the chemical is released. Chemicals could be deposited in an on-site RCRA-regulated, subtitle C hazardous waste unit, or in an on-site nonhazardous solid waste management unit. RCRA standards for hazardous waste units are, by regulation, designed to include technical controls to prevent release of contaminants into groundwater; if chemicals are placed in such regulated units, it is assumed that releases to groundwater are negligible. If chemicals are placed in nonhazardous land disposal units, we model the release of chemicals to groundwater. This analysis assumes that if the TRI form reports a RCRA ID number for the facility, then the on-site land releases are assumed to go to a RCRA hazardous waste regulated unit. Otherwise, the on-site land release is assumed to occur in a nonhazardous land disposal facility. This assumption introduces additional uncertainty to the analysis; some of the onsite disposal may go to a nonhazardous waste unit on the site. However, the TRI reports shed no light on this matter, and the magnitude of the uncertainty introduced is not known.

The TRI forms do not provide site-specific information that aids in the evaluation of groundwater transport, such as hydrogeological data. Unfortunately, these data are extremely site-specific and are not amenable to characterization by state or region of the country. Nonetheless, to maintain a concentration/exposure measure consistent with the approaches for direct air and water releases, we derive a surrogate dose using generic, conservative assumptions. This approach requires two steps: estimating leachate concentration (a measure of the amount of chemical that partitions from the waste to pore water) and estimating the dilution and attenuation of leachate from the disposal site to the well location.

Leachate concentrations can be estimated using a modeling approach with chemical-specific parameters. The general form of this estimate is as follows:

$$C_l = \frac{C_s \cdot 10^{-6}}{K_d}$$

where:

$C_l$	=	chemical concentration in leachate (kg/L),
$C_s$	=	chemical concentration in landfill solids (mg/kg),
$10^{-6}$	=	constant to convert (mg) to (kg), and
$K_d$	=	chemical-specific soil/water partition coefficient (L/kg).

Since we lack data about how materials are disposed onsite, all onsite land disposal is assumed to occur in landfills. It must be noted that the concentration in the leachate,  $C_l$ , must be compatible with the chemical-specific solubility (i.e. leachate concentration cannot exceed water solubility), so the smaller of the two values is used.

The average contaminant concentration in the landfill solids,  $C_s$ , can be estimated by dividing the total mass of contaminant disposed (converted from pounds per year to mg per year) by the total mass of waste disposed in the unit each year:

$$C_s = \frac{M_c}{M_w}$$

where:

$M_c$  = total mass loading of contaminant to landfill (mg per year), and  
 $M_w$  = total mass of waste disposed in landfill (kg per year).

The value for  $M_c$  is available in the TRI database; the value for  $M_w$  is a national number taken from an Agency source (EPA, 1988b). This report to Congress summarizes the distribution (by number of facilities and by industry type) of the tons per year of waste disposed in industrial nonhazardous solid waste landfills. Data are also reported for surface impoundments, waste piles and land treatment facilities. These summaries are reproduced in Appendix F.

Once leachate concentrations are estimated, the next step is to determine the magnitude of dilution and attenuation of contaminants that occur as the contaminant travels from the source to the well. The Office of Solid Waste (OSW) performed an analysis of dilution and attenuation of contaminants in groundwater during the development of the Toxicity Characteristic Leaching Procedure (TCLP) rulemaking (55 (61) *Federal Register* 11798). For that rule, OSW used Monte Carlo analysis to evaluate dilution and attenuation factors (DAFs) for 44 chemicals. In the Monte Carlo analysis, multiple iterations of a groundwater model were performed. For each model run, model parameter values were drawn randomly from their distributions.<sup>12</sup> The result of the analysis was a distribution of model results, where each model result was a DAF. OSW then selected the 85th percentile DAF for use in its regulatory calculations. For most chemicals modeled, the 85th percentile DAF was approximately 100. For this methodology, we use a DAF of 100 to estimate groundwater contaminant concentrations at the well due to contaminant leaching from on-site land releases. The concentrations are then used to calculate surrogate doses as shown below. Because OSW's DAFs do not reflect the effect of groundwater pumping on the concentration of chemicals in groundwater, the calculation of TRI surrogate dosages is oversimplified.

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<sup>12</sup>Distance to the well was one of the parameters varied in the analysis: the distribution of distance between a source and a well was derived from a survey of Subtitle D facilities.

$$C_{gw} = \frac{C_l}{100} \cdot 10^6$$

where:

$C_{gw}$	=	concentration in groundwater (mg/L),
$C_l$	=	concentration in leachate (kg/L)
100	=	dilution and attenuation factor (unitless), and
$10^6$	=	constant to convert (kg) to (mg).

The surrogate dose for exposure to contaminated groundwater from the facility is calculated as follows using standard exposure assumptions:

$$DOSE_{gw} = \frac{C_{gw} \cdot I_{water}}{BW}$$

where:

$DOSE_{gw}$	=	surrogate dose of contaminant in groundwater (mg/kg-day),
$C_{gw}$	=	concentration in groundwater (mg/L),
$I_{water}$	=	drinking water ingestion rate (L/day), and
BW	=	human body weight (kg).

The population exposed to contaminated groundwater is calculated from the number of persons receiving drinking water from groundwater within one kilometer of the facility. The population of persons served by well water is available for each county from the National Well Water Association data files. From these data, we can derive a “well water drinker” population density for each county (i.e., the percent of persons in the county who drink well water). This density is multiplied by the number of persons living within one kilometer of the landfill site to obtain the exposed population. [It is of course possible that chemicals migrate beyond one kilometer of the site, so this assumption may underestimate the population exposed. However, this is a typical distance for groundwater modeling that reflects the distances at which important parameters such as DAFs are derived. Confidence levels are lower at greater distances.] The Indicator Element for the groundwater pathway for the chemical is calculated by combining the surrogate dose, exposed population, and toxicity weight of the chemical. Off-site landfills are similarly modeled.

A summary of the values used in the groundwater calculation and the sources of these values appear in Exhibit 17. The approach to evaluating exposure from on-site land disposal for the Chronic Human Health Indicator is summarized in Exhibit 18.

#### EXHIBIT 17. Groundwater Modeling Parameters

Parameter	Value	Source/Comment
Concentration in leachate	calculated	mg/L
Partition coefficient	varies by pollutant	

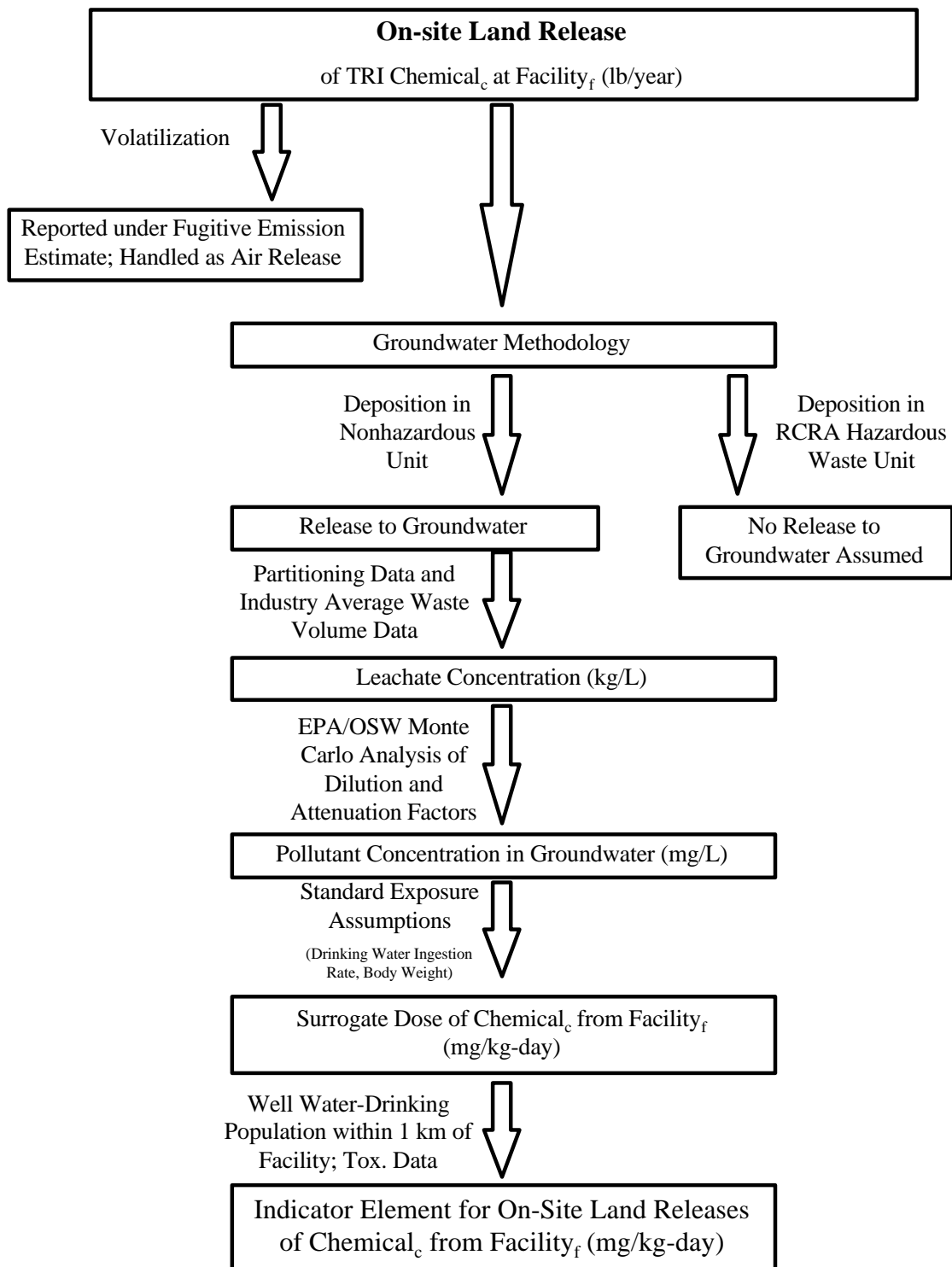
For the groundwater pathway, we use uncertainty category C, because the exposure estimate is based on a conservative, steady-state estimate of leachate concentration and on a conservative, generic dilution and attenuation factor.

#### Releases to POTWs

In 1991, 311 million pounds of TRI chemicals were discharged to the country's Publicly Owned Treatment Works (POTWs) compared with 271 million pounds discharged directly to surface waters. Modeling exposure from TRI discharges to POTWs requires: (1) location of the POTW to which the chemicals are discharged, (2) consideration of overall removal efficiencies of POTWs and resulting effluent discharges from POTWs, and (3) consideration of residuals management at POTWs:

- *Location of the POTW.* The latitude and longitude of POTWs receiving TRI transfers are not included in the TRI data base. However, the ZIP codes for the POTWs are available. For a given facility, the POTW is located on the grid based on the latitude and longitude of the ZIP code centroid.
- *Overall POTW removal rates.* POTWs cannot remove completely all of the chemicals in the influent; some of the chemical loading in the influent will be released in the POTW effluent. To calculate the fraction of transferred chemical removed by the POTW, the overall typical POTW contaminant removal rate for that chemical is applied to the transfer volume.
- *Partitioning within the POTW.* Chemical loadings may be removed by the POTW treatment processes through biodegradation, volatilization, and adsorption to sludge. Using average removal and partitioning rates, chemicals within POTWs are partitioned among effluent, biodegradation, air and sludge.

**EXHIBIT 18. Calculation of Surrogate Dose and Indicator Element from On-site Land Releases**



Various data bases and literature references were used to estimate typical POTW removal efficiencies and within-POTW partitioning rates for many TRI chemicals. The references and methods used for each chemical are described in Appendix D.

Once the fates of chemicals entering the POTW are estimated, the exposure levels associated with chemical loadings to each compartment will be estimated. Chemicals discharged in the POTW effluent are modeled using the surface water evaluation methods described above. Chemicals that biodegrade are assumed to degrade to chemicals that do not pose risk. POTW volatilization releases are treated like area-source air releases, as described above.

For chemicals that partition to sludge, the model used to estimate exposure should ideally depend on the sludge disposal method employed by the POTW. However, sludge disposal practices at a POTW receiving a TRI transfer cannot be determined from the TRI database. Therefore, the TRI Environmental Indicators algorithm currently models all POTW sludge as being landfilled at the POTW, a common method of sludge disposal. Landfilling of sludge is modeled as a land release using methods described above. Populations surrounding the POTW are modeled as the exposed population. POTWs may in reality use other methods of sludge disposal, such as incineration of sludge. If sludge were incinerated by a POTW, for example, this would result in different exposure levels and a different, larger exposed population.

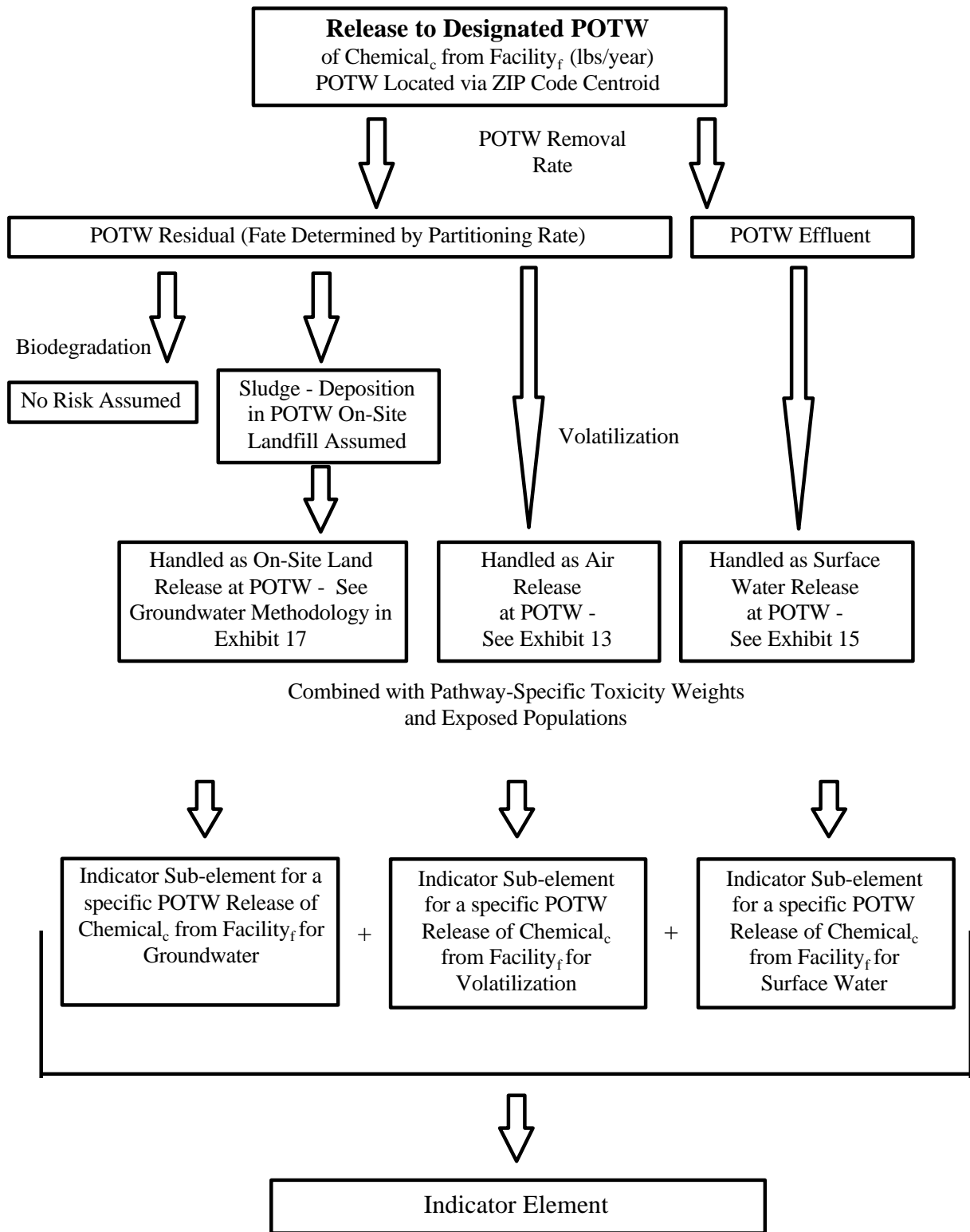
The uncertainty-adjusted indicator sub-elements from POTW effluent, volatilization at the POTW, volatilization of land disposed sludge, and groundwater contamination from land-disposed sludge are combined to yield a single facility-chemical-POTW transfer Indicator Element.

A summary of the approach to modeling POTW emissions used to calculate the Chronic Human Health Indicator is found in Exhibit 19.

### **Off-site Transfers**

In 1993, over 42 percent of TRI emissions were transferred to off-site locations for storage or disposal. TRI reporters are required to supply the name and address of the receiving facility. From these data, we must determine if wastes are sent to a hazardous or nonhazardous waste management facility. Submissions indicating transfer to a RCRA hazardous waste facility are not included in the Chronic Human Health Indicator; as described above, RCRA standards for hazardous waste units are, by regulation, designed to include technical controls to prevent release of contaminants into groundwater. If chemicals are placed in such regulated units, it is assumed that releases to groundwater are negligible. Therefore, only transfers to nonhazardous facilities are modeled.

# **EXHIBIT 19. Modelling of Exposure from POTW Releases**



As with POTW transfers, to assess the exposure potential associated with off-site transfers, we must have information about the off-site facility location and some of its characteristics. The ZIP code for the off-site facility is contained in the TRI data base; we locate the facility using the ZIP code centroid. Once we have located the off-site facility, the Indicators methodology requires: (1) the regulatory status of the unit to which the material is transferred, and (2) the treatment/disposal technologies used by the off-site facility.

The TRI forms require the reporting facility to indicate the treatment/disposal method used at the off-site facility. If this information is not reported (despite the requirement), the transfer is not evaluated in the algorithm, but is flagged as a missing value and assigned a zero.

Once the treatment method is established, we model exposure potential using the methods described above. If the treatment method is incineration, then destruction and removal efficiencies (DREs) are applied to the transfer amount. For organics, the DREs are assumed to be 99 percent, except for PCBs, which are assumed to have a DRE of 99.9999 percent, as required by TSCA regulation. For inorganics, values are taken from multiple hearth sludge incinerator studies (EPA, 1993). Once DREs have been applied, the releases are modeled using air modeling algorithms described above.

For off-site landfills, two major exposure pathways are considered. The groundwater pathway is modeled for off-site releases in the same manner as for on-site land releases. Volatilization, however, is modeled differently. For on-site releases, volatilization is included in reported fugitive emissions and thus exposure is modeled with on-site air releases. In contrast, for off-site land releases, volatilization emissions from land disposal must be estimated before exposure can be modeled.

The first step in estimating volatilization emissions is to estimate the concentration of chemical in the liquid phase (i.e., leachate). This equation was given earlier in the “On-site Land Releases” section:

$$C_l = \frac{C_s \cdot 10^{-6}}{K_d}$$

where:

$C_l$	=	concentration in leachate (liquid phase) (kg/L),
$C_s$	=	concentration in landfill solids (mg/kg),
$10^{-6}$	=	constant to convert (mg) to (kg), and
$K_d$	=	soil/water partition coefficient (L/kg).

The second step is to estimate the vapor phase concentration from the liquid phase concentration using the chemical's Henry's Law constant (the ratio of the chemical concentration in the vapor to the concentration in the liquid phase):

$$C_v = H C_l$$

where:

$C_v$	=	contaminant concentration in vapor phase (kg/L),
$C_l$	=	contaminant concentration in leachate (liquid phase) (kg/L), and
$H$	=	Henry's Law Constant (dimensionless).

Once the contaminant vapor concentration has been estimated, the flux of volatilizing contaminant may be estimated as:

$$Vol\ Flux = k_{vol} \cdot C_v \cdot 10^3$$

where:

Vol Flux	=	flux of volatilizing contaminant (kg/m <sup>2</sup> -sec),
$k_{vol}$	=	contaminant volatilization transfer velocity (m/sec),
$C_v$	=	contaminant concentration in vapor phase (kg/L), and
$10^3$	=	constant to convert (L) to (m <sup>3</sup> ).

The volatilization transfer velocity, or speed at which a contaminant is transported through a stagnant air layer immediately above the land disposal site, is taken from an EPA (1985) equation for uncovered landfills:

$$k_{vol} = \frac{0.17\ u\ (0.994)^{(T-20)}}{\sqrt{MW}}$$

where:

0.17	=	an empirical constant,
$u$	=	wind speed (m/s),
$T$	=	ambient air temperature (°C), assumed to be 15°C,
$MW$	=	molecular weight (g/mol), and
0.944	=	an empirical constant.

These formulae may be combined to express the volatilization flux as a function of the contaminant concentration in the solid phase:

$$Vol\ Flux = \frac{0.17\ u\ (0.994)^{(T-20)}\ H\ C_s\ 10^{-3}}{K_d\ \sqrt{MW}}$$

This flux estimate of volatilizing chemical is multiplied by an estimate of the area of the landfill to obtain an estimate of total emissions (mass per time). These emissions are then combined with weather data and data on populations surrounding the off-site disposal facilities to obtain population-weighted concentrations, using the same algorithms as those used for direct air releases from TRI facilities. Exposure uncertainty category C (that is, a factor of 10) is used for this pathway, because substantial assumptions and modeling are required to derive the exposure potential estimate. The data on population surrounding the off-site facility are extracted using the ZIP code of the off-site facility. Volatilization parameters are summarized in Exhibit 20.

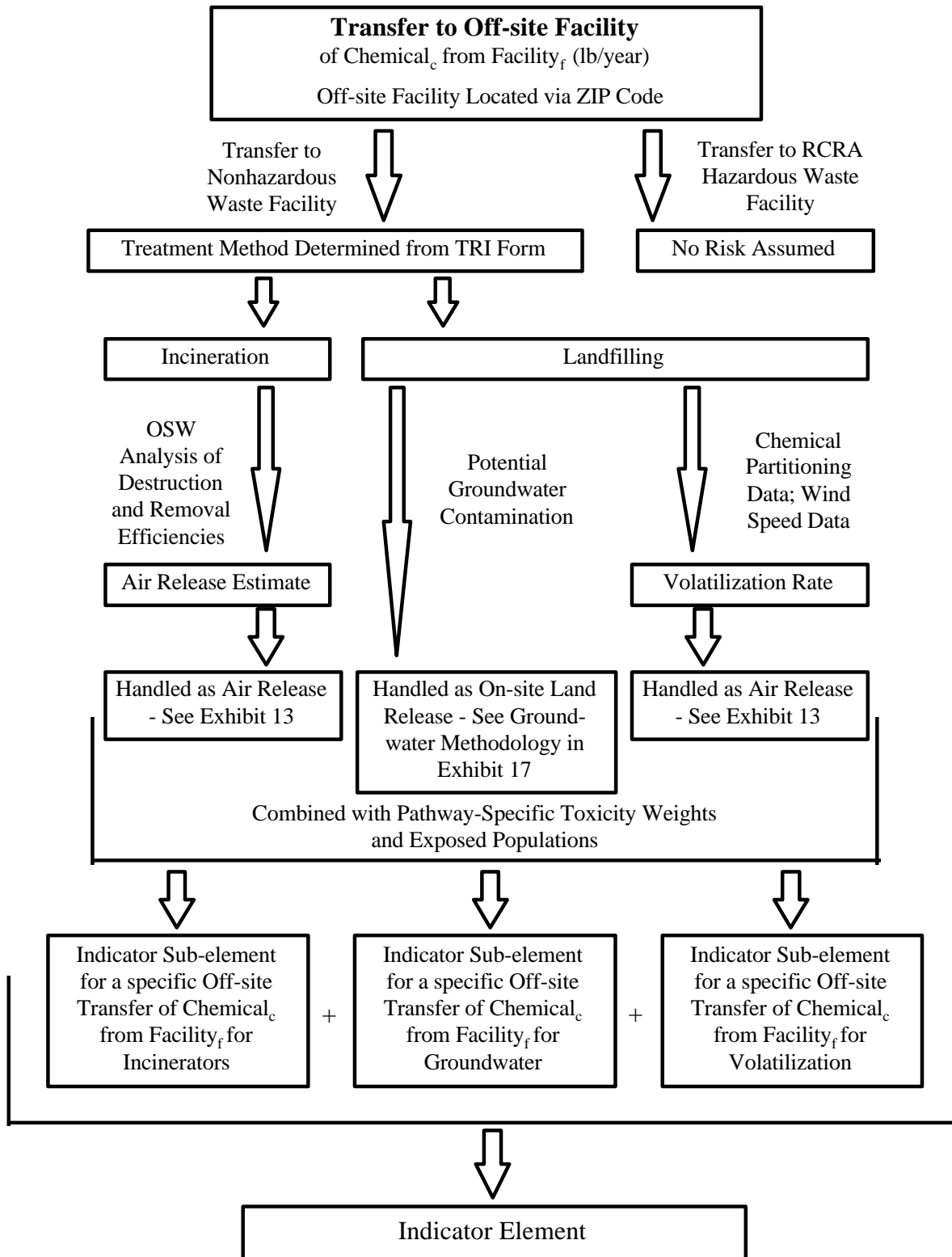
#### EXHIBIT 20. Volatilization Modeling Parameters

Parameter	Value	Source/Comment
$K_d$	varies by pollutant	Chemical properties database (Appendix D)
Molecular weight	varies by pollutant	Chemical properties database (Appendix D)
Henry's Law constant	varies by pollutant	Chemical properties database (Appendix D)
Average area of source: municipal solid waste landfill	32.5 acres	EPA (1988c)
Median area of source: industrial nonhazardous land disposal	landfill: 3 acres surface impoundment: 0.5 acres land treatment: 15 acres waste pile: 0.5 acres	EPA (1988d)
Mean wind speed	site-specific	m/s; from STAR data

The resulting sum of the uncertainty-adjusted indicator sub-elements from incineration, volatilization and groundwater exposures yields the facility-chemical-off-site transfer Indicator Element.

Exhibit 21 presents a summary of the method used to model off-site transfers.

## EXHIBIT 21. Modeling of Exposure from Off-site Transfers



## **EVALUATING ECOLOGICAL EXPOSURE POTENTIAL — GENERAL STRATEGY FOR AQUATIC SYSTEMS**

The estimated ambient water concentration value is used directly to evaluate potential exposures to aquatic life. The method for evaluating ambient surface water concentrations resulting from TRI releases is discussed above. Since the Chronic Ecological Indicator includes only one exposure pathway, there is no reason to use an uncertainty adjustment for cross-pathway uncertainty. Therefore, these surrogate values are used directly as the exposure potential for aquatic life.

### **V. METHODS TO ADJUST FOR SIZE OF POPULATION EXPOSED**

#### **ESTIMATING POPULATION SIZE AND REPRESENTING RURAL POPULATIONS**

Several options were considered for including the size of potentially exposed human populations in the Chronic Human Health Indicator. One option was to use the absolute population numbers, if reliable population data are available for an area. However, for small populations, the method uses rounded numbers rather than absolute numbers to avoid undervaluing potentially high impacts on rural populations. Using rounded numbers assures small populations of a minimum weighting. In effect, this inclusion gives more weight per capita to small populations.

For the air pathway, the Chronic Human Health Indicator method rounds exposed populations below 1000 persons up to a value of 1,000. For the surface water pathway, the minimum population size is 10, while for groundwater, the minimum population size is 1.

The determination of the size of the population exposed to TRI releases and transfers varies substantially depending on the medium to which the chemical is released. The methods for estimating the size of the exposed population are discussed for each pathway in chapter IV.

The method uses the most current Census population information (1990); thus, impacts to future populations are not modeled. For the groundwater pathway, modeled concentrations at the well could occur far in the future; in most cases, releases would not reach the point of exposure (i.e., the well) during the given year of TRI reporting. In this case, these future exposures are matched to the current population size. At present, the same population definition is applied to each year of TRI reporting, but project staff are attempting to define estimates of population between major (decennial) census dates.

Because of major difficulties in estimating sizes of the populations of ecological receptors, the TRI Ecological Indicator does not include a population weight. In effect, this approach assumes that all aquatic emissions occur in equally vulnerable locations. In actuality, the populations may differ among areas; thus, the Indicators method may either underestimate or overestimate impacts in a given area.

## VI. COMPUTING THE INDICATORS

This section of the report summarizes the actual computation of the TRI Environmental Indicators and the adjustments that will be made to the Indicators when chemicals or facilities are added to or deleted from the original set of TRI chemicals and facilities. The methods of calculating the Indicators are presented first; subsequent discussion focuses on methods to accommodate additions/deletions of both chemicals and facilities to the Indicators.

### INTEGRATING TOXICITY, EXPOSURE, AND POPULATION ADJUSTMENTS TO OBTAIN INDICATOR ELEMENTS

#### Chronic Human Health Indicator

The previous chapters described how each component of the Chronic Human Health Indicator (toxicity, exposure potential, population size) is developed as an input to the calculation of Indicator elements. The following equation shows how these components are combined to obtain a facility-chemical-medium specific element:

$$Indicator\ Element_{c,f,m} = Toxicity\ Weight_{c,m} \cdot Surrogate\ Dose_{c,f,m} \cdot Population_{f,m}$$

where:

c	=	subscript for chemical c,
f	=	subscript for facility f, and
m	=	subscript for medium m.

The components are multiplied because each component of risk (toxicity, exposure, and population) contributes in a multiplicative way to the overall magnitude of the impact. The result of the multiplication of the components is a facility-chemical-medium-specific “Indicator Element.” This element should be considered unitless, because each of the components (the toxicity weighting, surrogate dose and population) are all used as unitless weights, that are relevant only when compared to each other. It is reiterated that this unitless element is *not* a physically meaningful measure of quantitative risk associated with the facility, but is an approximate measure of relative risk impacts that is comparable to approximate measures for other facilities calculated using the same methods.

For chemicals with cancer effects, multiplying the weights associated with cancer toxicity and exposure to the chemical seems intuitive, since this is similar to the calculation of cancer risk with a slope factor or unit risk value and dose or exposure level. However, for chemicals with noncancer effects, the multiplicative nature of the toxicity and exposure weights may not seem intuitive, because in risk assessments, risk is usually characterized as the estimated exposure

divided by the RfD. However, because of the manner in which the toxicity weights have been constructed, the product of toxicity weight and surrogate dose varies in the same direction and degree as the ratio of exposure to RfD. This is because the toxicity weight is inversely related to the magnitude of the RfD. Thus, for a given exposure level, a chemical with a more stringent (i.e., lower) RfD will receive a higher Indicator value than a chemical with a less stringent (i.e., higher) RfD, as shown in the following example:

**EXHIBIT 22. Example of Weighting for Noncancer Effect**

	RfD (mg/kg-day)	Toxicity Weight	Surrogate dose (mg/kg-day)	Exposure/RfD Ratio	Toxicity Weight * Surrogate Dose
Scenario 1	0.1	10	1	$1/0.1 = 10$	$10*1 = 10$
Scenario 2	0.01	100	1	$1/0.01 = 100$	$100*1 = 100$

In addition, since no adverse effects are expected to occur below the RfD, one could argue that releases which result in surrogate doses below the RfD should be excluded from the Indicator. However, this approach was not pursued for the following reasons: first, the estimation of surrogate dose is only a crude approximation for the purposes of comparing one release to another in a relative way, and should never be considered an actual estimate of exposure. To exclude releases resulting in surrogate doses below the RfD would incorrectly imply that the method could predict precisely when doses would occur below the RfD. Second, exposure to the same chemical from multiple facilities, or multiple chemicals from one or more facilities affecting the same health endpoint could act additively to pose risk, even if each release individually did not result in an exceedence of the RfD. Finally, it should be kept in mind that if the surrogate dose is low, this will be reflected by a correspondingly low score relative to other releases for that chemical in the Indicator.

### **Chronic Ecological Indicator**

The methods for determining aquatic toxicity weight and surrogate dose were described in previous chapters. Again, effects on terrestrial wildlife are not considered in this Indicator. The following general equation combines these components for each facility and each chemical (only the water medium is evaluated):

$$\text{Indicator Element}_{c,f} = \text{Toxicity Weight}_c \cdot \text{Surrogate Dose}_{c,f}$$

where:

c = subscript for chemical c, and  
f = subscript for facility f.

As with the Chronic Human Health Indicator, the components are multiplied in this setting because each component (toxicity and exposure) contributes multiplicatively to the overall magnitude of the impact. The result of the multiplication of the components is a facility-chemical-water-specific “Indicator Element.” As with the Indicator Elements of the Chronic Human Health Indicators, these Chronic Ecological Indicator Elements should not be interpreted as actual quantitative measures of risk.

#### COMBINING ELEMENTS TO OBTAIN THE OVERALL INDICATORS

For both the Chronic Human Health Indicator and the Chronic Ecological Indicator, the overall Indicator value is calculated by combining the individual TRI chemical-facility-media Indicator elements. A simple sum of the component scores is used:

$$I = \sum \sum \sum E_{c,f,m}$$

where:

I = TRI Environmental Indicator of interest and  
E<sub>c,f,m</sub> = facility-chemical-medium-specific Indicator Element.

As many as 400,000 Indicator Elements for a given reporting year for the TRI will be summed to yield just one year’s score for a specific TRI Relative Risk-Based Environmental Indicator (e.g., the Chronic Human Health Indicator). In this method, each component score makes a contribution proportional to its size. The resulting Indicator value can be used in a number of ways, including tracking changes over time. For this purpose, one of the early years of TRI reporting is selected as the “base year” (e.g., 1988) and later years’ Indicator values compared to it. For the base year, the unitless score is scaled to a convenient round number such as 100,000 by dividing the base year Indicator value by itself and multiplying by 100,000; subsequent years’ data would be scaled by the same factor to provide a relative comparison. The magnitude of the final number to which the score is scaled depends on the size of the year to year change in the Indicator value, since very small changes in the basic Indicator would not be as discernable if the scaling number chosen for the base year is too small. It must be reiterated that while changes in scores over the years would imply that there have been changes in environmental impacts, the actual magnitude of the risk increase or decrease is unknown in absolute terms.

This approach considers together impacts from all types of health risks and exposure pathways. For example, impacts from releases for chemicals with cancer effects are not considered separately from those with noncancer effects. Because the Indicators model is a screening tool to be used for priority-setting, among other objectives, it is desirable to have an overall measure that integrates considerations of the impacts of releases, rather than having multiple disaggregated measures. However, the computer algorithm also allows the user to disaggregate the Indicator according to different attributes of the risk-related impacts. Therefore, particular users can examine different aspects of the impacts that are of interest to them.

### **Other Methods of Calculation Considered**

Alternative means of calculating the Indicators were considered, as discussed in Appendix G. Some of these included the arithmetic mean of the Element scores, the geometric mean of the scores, and the least-square difference of the scores. Each of these methods generates a score that will fluctuate as the individual components of the Indicator fluctuate. However, the methods do not produce readily interpretable results, and detecting fluctuations is less obvious than with more straightforward methods. To avoid aggregating element values to the point where important changes are not discernable, as well as for the greatest ease in calculation and interpretation, OPPT has concluded that the chemical-facility-media specific elements should simply be added and then adjusted to a manageable level.

### **USING THE INDICATOR APPROACH TO INVESTIGATE ENVIRONMENTAL JUSTICE ISSUES**

When calculating the full TRI Relative Risk-based Chronic Human Health Environmental Indicator, each Indicator Element is keyed to the facility from which the release is emitted, rather than the location where the impact of the release(s) occurs. The Indicator is designed in this manner so that all risk-related impacts from a given facility or set of facilities can be tracked. Because the Indicator is oriented toward tracking facilities, an analyst can use it to identify industrial sources that pose the relatively greater risk-related impacts, to examine changes in the performance of industrial sectors over time, and to suggest priority industrial sectors for further environmental management policies.

Another useful way to consider the impacts of TRI releases is to evaluate the total impacts from all facilities that affect a given geographic location. This orientation allows the analyst to assess risk-related environmental impacts of multiple releases on a given population. Combined with additional demographic information on affected populations, such as race, income, educational level, or age, the Indicator can be used to investigate environmental justice issues related to the distribution of environmental impacts across segments of the population.

When using the Environmental Justice Module to examine a defined geographic area, Grid Cell Elements are calculated separately for each location where the impact of a TRI release occurs. In the Indicator algorithm, the U.S. is divided into a grid of 1 km by 1 km cells: Grid Cell Elements are calculated for each release in each grid cell where an impact occurs<sup>13,14</sup>:

$$\text{Grid Cell Element}_{c,f,g,m} = \text{Toxicity Weight}_{c,m} \cdot \text{Surrogate Dose}_{c,f,g,m} \cdot \text{Population}_{g,m}$$

where:

c	=	subscript for chemical c,
f	=	subscript for facility f,
g	=	subscript for grid cell, and
m	=	subscript for medium m.

When using the Environmental Justice Module, the user has the option of examining discrete Grid Cell Elements, aggregated Grid Cell Elements or averaged Grid Cell Elements to investigate the relative risk-based impacts on either the defined population or, for comparative purposes, populations in distinct geographic areas.

To implement such calculations in the current version of the Indicators computer program, the analyst must first define a geographic area(s) of interest (creation of a subset is currently necessary because of computer memory limitations). The defined geographic area can measure up to approximately 2500 km<sup>2</sup>.

Once the geographic area of interest is defined, the model looks for facilities within the defined region, and any facilities 10 km outside the border of the defined region in any direction. The 10 km distance is used because it is the current distance to which air releases are modeled within the Indicator computer model. By including facilities within a 10 kilometer buffer, the model can account for air releases originating outside of the defined region but affecting cells within the defined region. In this instance, the term “facility” refers to both TRI reporting facilities, and any facilities that receive transfers from TRI reporting facilities, such as POTWs or waste treatment facilities. The Grid Cell Elements are then calculated for each grid cell-facility-chemical-medium combination. Summing across chemicals, facilities and media for each grid cell gives a value representing the total risk-related impacts in that grid cell.

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<sup>13</sup>The sum of the Grid Cell Elements for a given chemical release to a single media by a single facility would equal the Indicator Element routinely calculated by the Indicator algorithm.

<sup>14</sup>For those instances when Grid Cell Elements are to be exported for use in a GIS model containing a census data base the population weight is omitted.

This description of the Environmental Justice Module applies only to investigation of impacts from air releases, and transfers that result in air emissions, but the capability for evaluating impacts of additional release media can also be developed. The computer algorithm is currently being revised to include the capability to investigate environmental justice issues related to air impacts, and may be revised later to include other pathways.

## **SCALING THE INDICATORS FOR CHANGES IN TRI REPORTING**

When a change occurs in the number of chemicals and facilities represented in TRI, the numerical value of the Indicators will certainly be altered if no adjustments are made to the method of calculation to account for the changes. However, such changes would not necessarily represent a sudden change in actual environmental impact, but rather would reflect a broader understanding of the impacts that had existed all along. To maintain comparability in the Indicators' scores over time, the Indicators would have to be adjusted in some manner when such modifications in reporting occur.

A change in the number of chemicals and facilities in TRI can occur through several mechanisms. First, the addition to or deletion of chemicals from the TRI chemical list will occur as EPA responds to petitions or initiates its own action through the chemical listing or delisting process. Several additions and deletions to the dataset have already occurred since 1987, the first year of TRI reporting. Furthermore, as mentioned earlier, in November 1994, the Agency added 245 chemicals and chemical categories to the TRI chemical list, effective for the reporting year 1995. The deletion of chemicals would presumably have a minor effect since such chemicals would be deleted due to their low risk; these chemicals are likely to make only a minimal contribution to the Indicators.

Compliance with TRI reporting has improved over time. Effective for the 1998 reporting year the addition of certain SIC codes to TRI has also been approved, adding to the universe of reporting facilities<sup>15</sup>. Increases in the number of reporting facilities may also occur as a result of changes in reporting requirements. For instance, in first two years of reporting, facilities that manufactured or processed more than 50,000 pounds were required to report their releases. However, EPCRA lowered this threshold to 25,000 pounds in 1989. All of these modifications can act to alter the total emissions reported under TRI and the Indicator's estimate of the associated relative risk-based impacts.

To account for changes in the representation of chemicals and facilities in the TRI data base, the TRI Environmental Indicators method may create new Indicators when significant new

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<sup>15</sup>This facility expansion rule will require the affected facilities to report their releases in the year 2000 for the 1998 reporting year. The affected SIC codes are: codes 10 (except 1011, 1081, and 1094), 12 (except 1241), industry codes 4911, 4931 and 4939 (limited to facilities that combust coal and/or oil for the purpose of generating power for distribution in commerce, 4953 (limited to facilities regulated under RCRA), 5169, 5171, and 7389 (limited to facilities engaged primarily in solvent recovery services on a contract or fee basis) (U.S. EPA 1997a).

additions are made to the TRI chemical list. “Significant” additions could be several minor additions that have been made over the course of a few years that eventually constitute a significant change, or a single major influx of new chemicals (due to Congressional or Agency action, for example). These new Indicators would include both old and new chemicals and facilities. However, to track trends for the initial set of chemicals and facilities, EPA would also retain a separate Indicator consisting of only the “original” facilities and chemicals. The Work Group considered a variety of other options to adjust for additions to the set of chemicals and facilities; details of these options, and their advantages and disadvantages, are found in Appendix G.

While deletions from the TRI chemical list probably would not result in any significant change to the Indicator value in most cases, the possibility of a change in Indicator value due solely to deletions in the year the deletion takes effect, makes adoption of adjustment methods important. Thus, when major deletions occur, the Indicator will be recomputed, excluding deleted chemicals in all years.

Finally, the yearly TRI reporting data for a given list of chemicals and facilities are the subject of ongoing quality control review and revision. As a result, yearly comparisons could be flawed if ongoing revisions by individual facilities were not included in each year’s Indicator. Therefore, the TRI Environmental Indicator will be recomputed for all years in the data base on an annual basis in order to incorporate revisions to the reporting data.

## **GENERATING “SUBINDICATORS”**

In addition to computing an overall Indicator, the individual Indicator Elements can be combined in numerous other ways for further analysis. The detailed calculations used to create the Indicator Elements allow computation of “subindicators” for individual chemicals, geographic regions, industry sectors, facilities, exposure pathways and other parameters. These subindicators, like the overall Indicator, cannot be compared to some absolute level of concern, but can help identify the relative contribution of various components to the overall estimate of relative risk-based impacts of emissions. The ability of users to create these “subindicators” makes the TRI Environmental Indicators system a powerful tool for risk-based targeting, prioritization and policy analysis.

## **VII. CURRENT IMPLEMENTATION OF THE INDICATORS METHOD**

### **COMPUTER PROGRAM TO CALCULATE THE INDICATORS**

The TRI Chronic Human Health Indicator is currently implemented in a Microsoft Windows-based, stand alone PC computer program. The program allows users to calculate the overall Chronic Human Health Indicator for all years of data and to present the results in various graphical and tabular formats, as well as save selected data to spreadsheet and data base formats

(e.g., Microsoft Excel and dBase). The computer program also allows the users to specify particular subsets of data, for the creation of “subindicators.” The program includes on-line help for all of the program functions. The program will be documented in the [TRI Environmental Indicators computer program documentation]. A User’s Guide will also be made available.

## **CHEMICALS AND FACILITIES CURRENTLY INCLUDED IN THE INDICATORS**

Conceptually, the Indicators method is intended to include all chemicals that are reportable to the Toxics Release Inventory. However, for the current version, some chemicals are excluded because they have not yet been assigned toxicity weights (many of those have little or no reported emissions) or are missing physicochemical data. Currently 345 of the 656 TRI chemicals listed as of the 1995 reporting year have been assigned toxicity scores; 296 of these are based on IRIS and HEAST values and 49 based on expert review within OPPT. Scoring for all of the current TRI chemicals is discussed in the Toxicity Weighting Summary Document (EPA, 1997) and is summarized in Appendix C of this document. The evaluation of TRI chemicals with regard to aquatic toxicity will have to be conducted when the TRI Ecological Indicator is implemented.

In designing the TRI Chronic Human Health Indicator method, the use of a subset of chemicals and/or facilities was considered. There may be reasons to exclude certain facilities from the Indicators. For example, the reliability of reporting from certain facilities may be questionable. There may also be concerns about the resource and computing requirements for including all facilities in the Indicators. Ultimately, based on the recommendation of the peer reviews, the Work Group decided to include all facilities emitting chemicals reportable to the Toxics Release Inventory, since there were substantial difficulties in ensuring the selection of a representative set of facilities.

## **VIII. ISSUES FOR FUTURE CONSIDERATION AND CONCLUSIONS**

There are two general types of issues to consider for future effort: specific methodological issues for the Indicators developed to date, and development of additional Indicators. The methodological questions associated with the Indicators developed to date include the following:

- how to compute the Acute Human Health and Acute Ecological Indicators given the current reporting under TRI;
- extending the Ecological Indicator beyond consideration of only aquatic life;
- whether severity of effect should be considered in the toxicity score for a chemical;
- for off-site transfers, how to better match TRI transfers to particular treatment practices (e.g., which TRI chemicals are sent to hazardous or nonhazardous waste management facilities; or which specific treatment practices are used at which POTWs);

- how to incorporate information and/or estimates on changes in population for each year rather than using 1990 Census data for all years; and
- how to estimate the potential impact of non-landfill, non-incineration treatment (e.g., land application).

The flexibility of the current TRI Environmental Indicators method and computer program allows accommodation of data from other sources besides the TRI data base. With additional data, the system could be used to develop additional Indicators that provide information on measures of environmental impacts other than risk alone. For example, an Indicators model that explicitly incorporates consideration of environmental justice issues is being developed using the TRI Relative Risk-Based Chronic Human Health Indicator as the foundation.

Appendix H discusses expanding the TRI Environmental Indicators to reflect indirect health and environmental impacts from TRI chemicals, such as global climate change, acid deposition, stratospheric ozone depletion, tropospheric ozone formation, and particulate deposition. While many of these impacts have health-related effects, the complexity and uncertainty in modeling them may make it impossible to incorporate them into the present set of Indicators.

As an indication of improvements in environmental quality over time, the TRI Environmental Indicators will provide EPA with a valuable tool to measure general trends based upon relative risk-related impacts of TRI chemicals. Though these Indicators do not capture all environmental releases of concern, they do generally relate changes in releases to relative changes in chronic human health and ecological (aquatic life) impacts from a large number of toxic chemicals of concern to the Agency. Importantly, the Indicators also provide an ability to analyze the relative contribution of chemicals and industrial sectors to environmental impacts, and serve as an analytical basis for setting priorities for pollution prevention, regulatory initiatives, enforcement targeting and chemical testing.

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## **Appendix A**

### **Survey of Ranking and Scoring Systems**

## I. Survey of EPA Scoring and Ranking Efforts

Scoring and ranking of chemicals is not a new undertaking. Numerous efforts have focussed on categorizing and ranking chemicals for a number of purposes. The most common purpose is devising a methodology to choose from among a vast number of chemicals those that merit further scrutiny. The following is a review of sixteen EPA scoring and ranking systems that have been or are used by OTS and other Agency Offices.

### A. OTS Efforts

#### 1. Screening Methodology for Pollution Prevention Targeting

USEPA (date unknown), Prepared for the Office of Toxic Substances

The Office of Toxic Substances prepared a screening methodology as a tool for targeting chemicals for pollution prevention. A three step scoring system, based on the toxicity (both potency and type of risk posed) and on the release/production ratio of the chemical, was used. Several risk classifications were evaluated; within each classification, a chemical was given a preliminary score of 3, 2, or 1 for high, medium, or low concern, respectively. The first risk area evaluated was cancer potency. All chemicals designated as B2 carcinogenic were given a preliminary score of 3 (high). Oncogenicity received an additional weighting factor of 3 to arrive at a raw score for cancer potency. General chronic toxicity and ecotoxicity were scored; these scores were given an overall weighting factor of 2. Reproductive effects, neurotoxicity, and developmental toxicity were also scored, but these scores were given a weighting factor of 1. The raw scores for all four risk groups were added together and multiplied by the release/production ratio to arrive at a composite score. For each chemical the composite score was calculated as:

$$CS_i = (O_i \cdot 3 + RDN_i \cdot 1 + C_i \cdot 2 + E_i \cdot 2) \cdot \frac{Release_i}{Production_i}$$

where:

$CS_i$	=	Composite score for chemical <i>I</i>
$O_i$	=	Oncogenicity concern for chemical <i>I</i>
$RDN_i$	=	Reproductive, developmental, neurotoxicity concern for chemical <i>I</i>
$C_i$	=	Chronic toxicity concern for chemical <i>I</i>
$E_i$	=	Ecological toxicity concern for chemical <i>I</i>

This methodology was used for internal EPA chemical targeting. It has not been, to our knowledge, publicly reviewed.

Pros: Method is simple. Broadly accounts for potency and severity of risk posed. Having three broad categories of potency allows the use of structure-activity and professional judgment to score chemicals lacking extensive toxicological databases. Includes consideration of both cancer and noncancer effects.

Cons: Method groups chemicals very broadly, limiting the variation in potencies that can be expressed. Method ranks chemicals ordinally, not proportionately, which does not allow for accounting of the magnitude of differences among the chemicals. Does not have an exposure component. Assumes that carcinogenic effects are more serious than reproductive effects. To our knowledge, method has not been reviewed outside of the Agency.

## **2. TSCA's TRI Chemical Risk Assessment Pre-screening Methodology**

USEPA (date unknown), Memo from the Office of Toxic Substances (date unknown)

The objective of this exercise was to select the most likely candidates among TRI chemicals for possible regulation under TSCA. Of the 309 TRI chemicals, 193 were eliminated outright because they were already being assessed or regulated by another EPA division, they were not subject to TSCA, or no reports of use were received by EPA.

The remaining 116 chemicals were preliminarily ranked by exposure assessment and hazard assessment. The two assessments were used in concert with the investigators' knowledge to judge which chemicals presented the most significant risks to human health. This group of roughly 20 chemicals received top priority for more extensive and rigorous investigation, including exposure and hazard assessments, to determine which of them should be considered for regulation under TSCA.

### **Preliminary Exposure Ranking**

One hundred sixteen TRI chemicals were ranked using the Exposure Scoring System for Existing Chemicals. The system was used to rank each chemical in four pathways: surface water (drinking water), environmental (aquatic organisms), ambient air, and groundwater. These rankings were not combined in a final ranking. To perform the rankings, two measures were estimated in each pathway for each chemical.

The first measure, potential of exposure, is a measure of the presence of the chemical in the environment. If the chemical is not expected to be released to a particular pathway, it is assigned a score of "none" for no potential of exposure. Otherwise, if the chemical does not exceed thresholds for physical and chemical properties (half-life, Henry's Law constant, vapor pressure), it is assigned a "low" or "none". Those that are expected to be released in a particular pathway and exceed the thresholds are assigned "high", "medium", or "low" potential of exposure depending on the level of potential exposure that is calculated by the program. This calculation is a function of release and concentration levels at sites. Rough estimates are used if only partial information is available.

The second measure, population, is a score of the number of people that might be exposed to the chemical. It is calculated for each pathway and chemical. The system simply adds up the populations surrounding production sites, or if exposure mostly occurs during industrial use, extrapolates exposed populations from the number of industrial use sites. The final "high/medium/low/none" score is based on population thresholds.

The final score for each pathway area uses the following determination matrix:

Final Exposure Score		Population Measure			
		High	Medium	Low	None
Exposure Measure	High	High	High	Medium	None
	Medium	High	Medium	Low	None
	Low	Medium	Low	Low	None
	None	None	None	None	None

### **Preliminary Hazard Ranking**

EPA intended to develop a Hazard Ranking System to rank the TRI chemicals based on measures of toxicity. However, only a preliminary search system was developed. It allowed the user to score all TRI chemicals that fit given criteria, e.g. all those with an RQ over 1000 lbs. This system was used to develop simple lists of high toxicity chemical groups. Using this information and their best judgement, the pre-screeners selected roughly 30 chemicals which they determined to be the most hazardous.

Note that this ranking system has only been used within EPA's Office of Toxic Substances and has not been publicly reviewed.

Pros: Exposure screening includes four pathways of exposure. Modelling approach is used to evaluate exposure potential. Population surrounding TRI site is also included as a measure of exposure potential.

Cons: Although modelling is used for exposure evaluation, the results are used to group the chemicals into low, medium and high exposure potential groups. Pathway-specific scores are not combined, thus requiring further judgments to evaluate overall exposure potential of a chemical. To our knowledge, method has not been reviewed outside of the Agency.

### **3. Chemical Scoring System for Hazard and Exposure Identification**

O'Bryan, T. R. and Ross, R. H. (1988) Journal of Toxicology and Environmental Health, Vol (1):119-134

This system was developed by the Office of Toxic Substances and by the Oak Ridge National Research Laboratory. It combines expert judgement and objective scores to screen chemicals for further investigation for potential regulation under TSCA. Chemicals are scored in eleven areas:

Oncogenicity	Genotoxicity
Developmental toxicity	Acute and chronic mammalian toxicity
Aquatic toxicity	Bioconcentration
Chemical production volume	Occupational exposure
Consumer exposure	Environmental exposure
Environmental fate	

Scores are assigned by and reconciled between two independent experts. While the scores are based on delineated parameters, they can be adjusted in accordance with expert opinion. Scores for oncogenicity, genotoxicity, developmental toxicity and the exposure measures are based on weight-of-evidence. Scores for the others are based on thresholds (e.g. a bioconcentration score of 9 is assigned for BCF levels above 1000.) Tables 1 through 3 in our August 26 memorandum delineates the numerical ranges that comprise these scoring methods. In some cases, structure activity relationships were used to supplement available data. Individual scores generally range from 0 to 10 and are intended for comparison across areas and chemicals but not as weights for the calculation of a final chemical score. In fact, the methodology does not develop a final score. Instead, the scores from all eleven areas are presented as a score profile to which expert judgement is applied to determine whether a chemical presents a great enough hazard to undergo further investigation under TSCA. Note that this methodology has been published in a peer-reviewed journal.

Pros: System considers a large number of health endpoints (cancer, developmental toxicity, genotoxicity) in the evaluation. Makes use of both available data and expert judgment, allowing for coverage of a large number of chemicals. Published in a peer-reviewed journal.

Cons: System does not combine scores for overall judgment on relative toxicity of a chemical. In fact, the method explicitly states that scores can be used for comparisons across areas, but are not intended as weights for combination into a final score. Method does not include an exposure component.

#### **4. CERCLA Section 104 "Third Priority List" of Hazardous Substances that will be the Subject of Toxicology Profiles**

USEPA 1990, Prepared for the Office of Toxic Substances, February

EPA is using this system to select and rank the 275 most hazardous chemicals from among all substances found at National Priority List sites. Three principal criteria determine how hazardous a chemical is: 1) frequency of occurrence at NPL sites, 2) chemical toxicity, and 3) potential for human exposure. Measures of these criteria are used to calculate site and exposure ranks for each chemical, which determine the chemical's final ranking.

Frequency of occurrence is measured as the percent of sites at which the chemical is known to occur. Toxicity of the chemical is measured by its Reportable Quantity (the lowest of the mammalian, acute and chronic toxicity RQs was used.) When these ratings were not available, the chemical was assigned an RQ equivalent by the EPA Structure Activity Team. A site index was calculated for each chemical as:

$$\text{Site Index} = \frac{\text{Frequency of occurrence (percent)}}{RQ}$$

The chemicals were assigned ordinal site ranks beginning with 1 for the chemical with the highest site index, 2 for the chemical with the next highest site index, etc.

The measurement of chemical exposure is considerably more involved. First, an exposure index value is calculated for each chemical as:

$$\text{Exposure index} = WCR + WFR + SCR + SFR + (2 \times BPR)$$

where:

<i>WCR</i>	=	the geometric mean of chemical concentration in water at all sites where the chemical occurred, ranked ordinally
<i>WFR</i>	=	percent of sites at which the chemical occurred in water / percent of sites at which the chemical occurred in any media, ordinally ranked
<i>SCR</i>	=	the geometric mean of chemical concentration in soil at all sites where the chemical occurred, ranked ordinally
<i>SFR</i>	=	percent of sites at which the chemical occurred in soil / percent of sites at which the chemical occurred in any media, ordinally ranked
<i>BPR</i>	=	boiling point of the chemical, ordinally ranked

For WCR, the geometric mean as indicated is calculated for each chemical. The chemicals are then ranked ordinally according to this value; WCR equals the rank assigned to the chemical.

This method holds for each of the five variables listed above. Note that boiling point values are used as a correlate of potential for air migration.

Because NPL site concentration data are not available for many chemicals, a second methodology to calculate exposure was developed to complement the first. This method takes advantage of the fact that a chemical's status as a chemical of concern gives some indication of the chemical's exposure potential. Thus chemicals were ranked ordinally by the number of NPL sites at which they were listed as chemicals of concern. The lesser of this measure and the exposure index described above was used as the exposure rank.

Finally, these ranks were adjusted based on existing exposure information compiled in six data bases: NRC, AHE, DOT/HMIS, NEXIS, NHATS and RTS. Because of source and methodological disparities between the databases, the data they contained were not in themselves useful. However, because the simple occurrence of a chemical in one of the databases implies some degree of exposure, the number of databases in which a chemical was listed was used to determine the adjustments made to the exposure ranks. (Note that because the first four databases contained data from overlapping sources, multiple occurrences of a chemical in these databases was taken as a single listing.) The adjustment was made as follows. The exposure rank was multiplied by a factor of 0.9 if a chemical was listed in only one database, by 0.8 if in two databases, and by 0.7 if in three databases.

The site and exposure ranks of each were combined using the following formula:

$$\text{Hazard Index} = 2/3 \times \text{Site Rank} + 1/3 \times \text{Exposure Rank}$$

The weights reflect the fact that the site rank represents two of the three principal criteria mentioned initially, while the exposure rank represents only one. The chemicals were assigned final ordinal hazard ranks beginning with 1 for the chemical with the lowest hazard index, 2 for the chemical with the next lowest site index, etc.

Pros: Uses a peer-reviewed, well-established measure of relative toxicity (RQ) for toxicity ranking. Combines all measures (toxicity, exposure, frequency of occurrence) into a single index for each chemical.

Cons: Exposure component relies on availability of site-specific concentration data for exposure potential evaluation, which is not available for our purposes. Toxicity and exposure ranked ordinally, so that proportional differences in potency and exposure potential are not captured. Use of RQ also does not capture severity of effects.

## **5. Toxic Chemical Release Inventory Risk Screening Guide**

USEPA 1989, Prepared by the Office of Toxic Substances, Volume 1, July

The Risk Screening Guide serves to explain both the meaning of Toxic Release Inventory (TRI) data and ways of interpreting that data. Volume One of the document is divided into five

sections. The first section details the advent of the TRI program as well as the nature of, limitations on, and modes of access to the TRI data. Section Two details and explains the elements of risk assessment. Section Three presents the guide's qualitative methodology for risk assessment for each exposure route, incorporating the elements detailed in Section Two. Section Four proposes options for acting on the results of the assessment and Section Five lists a host of resources that can be used to answer any further questions.

The Risk Screening System presented in Section Three merits special attention. The system centers itself around qualitative measurements of different chemical-specific and site-specific factors. The user of the system first selects an exposure route (either air, land, surface water or POTW). The next step is to record the location of release, the zones of effect (inner and outer), and the population of interest. The user then delineates different "exposure factors" which depend upon the exposure route chosen (i.e. wind direction for air or bioconcentration factors for surface water). The scores for these factors depends upon the factor being discussed. For example, a water discharge receives a "+" if it flows to a small lake or stream and a "-" if it flows to a large body of water. Next, the user should select a toxic measure for each chemical from among a set of measures presented in Appendix A (discussed below). The user selects the lowest ranking among all of the different toxicological ranks. Next, the quantity of release should then be listed as either "high," "moderate," or "low" through the use of data presented in Appendix C. The user compares the releases as recorded in TRI to either the table of median emissions or by to local releases. Exposure factors should then be recorded as detailed in Appendix D (discussed below), including high/low environmental transformation, release rate, and any other factors which may seem relevant.

The result of the risk screening system is a profile of scores. From this information it is possible to assess the relative severity of industrial practices in the area. The user can consult local experts in order to get a feel for the individual risk.

Volume Two includes appendices which provide data and examples to facilitate the assessment process. Appendix A ranks toxicological information on chemicals according to the following scheme:

Toxicological Measure	Group 1	Group 2	Group 3
TPQ (lbs.)	1 10 100	500	1,000 10,000
RQ (lbs.)	1 10 100	1,000	5,000
RfD (mg/kg-day)	< 0.01	0.01 - 0.1	>= 1.0
WQC (mg/L)	< 1	1 - 10	>= 10
Cancer Potency	All		

These ranking boundaries are used for each of the RQs (aquatic, chronic, acute, and carcinogenic), RfDs (inhalation and oral), and WQCs (chronic and acute).

Appendix B aids users in assessing air releases. It discusses a generic air modelling exercise which uses the Industrial Source Complex Long-Term (ISCLT) model. It provides two graphs which display the results of generic model runs, the first plotting concentration versus distance from the release site for various stack heights, and the second plotting concentration versus distance from the release site for various durations of release. Multiplying data points on the graph by the actual release quantities provides an estimate of the concentration at different distances of concern.

Appendix C assists users in assessing the severity of chemical releases. It provides information on median chemical release data and actual TRI chemical release data (classified by SIC code) to assist in assigning a "severe," "moderate," or "low" score to the quantity of release (see the discussion on the Risk Screening System in Volume One).

Appendix D provides information on environmental fate characteristics of different chemicals to provide rankings. The characteristics used to evaluate fate in different environmental media and their rankings are listed below:

Factor	Measure	High Concern (+)	Low Concern (-)
Volatilization	Henry's Constant (atm-m <sup>3</sup> /mol)	$\geq 10^{-2}$	$\leq 10^{-6}$
Leaching & Soil Mobility	Log <sub>10</sub> (K <sub>oc</sub> )	$\leq 1.5$	$\geq 4.5$
Bioconcentration	BCF	$\geq 1,000$	$\leq 250$
Air Abiotic Persistence	Atmospheric Half-life	$\geq 1$ year	$\leq 1/2$ day
Water Abiotic Persistence	Aquatic Half-lives	$\geq 1$ year	$\leq 1/2$ day
Air Biotic Persistence	Degradation Rate	many months to years	1 to 7 days
Water Biotic Persistence	Degradation Rate	many months to years	1 to 7 days
Biological Treatment	Rate of removal in bio. treatment	Log <sub>10</sub> (K <sub>ow</sub> ) $\leq 1.5$ H <sub>c</sub> $\leq 10^{-5}$ resistant to degr.	rapidly removed: -P for phys/chem -B for biodegr.

The measure for water abiotic persistence stems from the longest of the hydrolysis, direct photolysis, and indirect photoreaction.

Appendix H presents and describes the Roadmap database as well as other databases that contain information on Section 313 chemicals. The Roadmap database includes the following information for each chemical in tabular form:

- ! Federal regulations that apply to the chemical, along with relevant regulatory levels
- ! States that have drinking water standards or recommendations, along with relevant regulatory levels, as reported in the Federal-State Toxicology and Regulatory Alliance Committee (FSTRAC)
- ! States that have ambient air information, including ambient air standards or guidelines, pollutant research information, source testing information, monitoring data, emissions inventory information, and permitting information, as reported in the National Air Toxics Information Clearinghouse (NATICH).

- ! States that have water monitoring information, as reported in the Storage and Retrieval Systems (STORET).
- ! General sources of information, including on-line data bases, and documents from EPA and other sources.

This appendix includes expanded descriptions of these information sources. ROADMAPS has since been updated to include additional data. Its "Carcinogenicity Matrix" includes results from the National Toxicology Program bioassay tests (either positive or negative for carcinogenicity); the National Toxicology Program's carcinogenicity ranking; the carcinogenicity rating assigned by the International Agency for Research on Cancer; the EPA's carcinogenicity rating; and the GENETOX carcinogenicity evaluation. It also now contains a "Health and Environmental Effects" table which indicates whether a chemical is at a level of concern for heritable mutations, developmental toxicity, reproductive toxicity, acute toxicity, and chronic toxicity, as well as the references for this data (among EPA databases).

The remaining appendices contain other information to guide a use through the risk assessment process. Appendix E presents information concerning the different types of releases, the release frequency, existing controls, and estimation methods for the releases. Appendix F presents a case study using the risk screening method (described below). Appendix I presents a sample EPA Hazardous Substance Fact Sheet. Each of these sheets discusses one of the Section 313 chemicals, providing information on typical modes of exposure, means of protection, proper handling, etc. Appendix J provides an example of an EPA Chemical Profile which provides physiochemical information on the Section 313 chemicals and which also discusses topics covered on the EPA Hazardous Substance Fact Sheet.

Pros: Appendix A of the Risk Screening Guide allows grouping of chemicals according to any of five measures of toxicity; using alternative measures of toxicity allows a larger number of chemicals to be scored than if only a single measure was used. Appendix D groups chemicals into groups of "high concern" and "low concern" based on environmental fate characteristics. The Risk Screening Guide has been peer reviewed and is published.

Cons: The grouping approach allows only broad characterization of toxicity and exposure, and does not consider severity or potency. Exposure evaluation does not explicitly consider populations (although this can be considered on a site-by-site basis).

## **B. Other Agency Scoring Systems that Use TRI Data**

### **1. Targeting Pollution Prevention Opportunities Using the 1988 Toxics Release Inventory**

USEPA 1990, Prepared for the Office of Policy, Planning and Evaluation, Pollution Prevention Division, September 29

OPPE's Pollution Prevention Division (PPD) developed a method to rank chemicals and facilities based on total volume of a subset of TRI chemicals. A list of high-priority chemicals was established for air, land, and water releases based on toxicity and exposure potential (based on the mobility of the chemical) in the TRI Risk Screening Guide. After a list was established for each media, the release volume of those chemicals became the ranking instrument. While no exposure-based adjustments were actually made to the rankings, possible methods for such adjustments were discussed in some detail in the text. The population considered at risk for each pathway varies by the mobility of the chemical. Thus, only populations relatively close to the facility are considered for low mobility chemicals, while at greater distances are included for high mobility chemicals. The table below shows how distance from facility and chemical persistence affect PPD choice of populations. PPD also proposed a method to adjust for the exposure potential of aquatic ecosystems for discharges to surface waters. Similar to human populations within circles of given radii from the facility, the stream volume acts as a proxy for aquatic exposure. The water-volume proxy assumes that densities and types of aquatic organisms are constant among all streams and are strongly positively correlated with total volume of water. Proposed methods for accounting for ecological risk from discharges to other media were resource intensive and did not lend themselves to computer automation.

This method was used for internal EPA chemical evaluation and has not been publicly reviewed.

#### **Concentric Ring Radius From Facility For Population Count**

Pathway	Mobility of Chemical		
	High	Medium	Low - No Data
Point and Non-Point Air Release	4 miles	2 miles	1 mile
Underground and Land Releases	1 mile	1/2 mile	1/4 mile
Surface Water Releases	15 miles	10 miles	5 miles

**Note:** Surface water distances are downstream distances from the facility.

Pros for exposure evaluation: Combines Risk Screening Guide environmental fate groupings with simple rules for defining the size of the potentially exposed population. This is a straightforward approach that allows quick, rough weighting of emissions by potential exposure.

Cons for exposure evaluation: Does not consider factors affecting differences in media concentrations among sites as part of exposure evaluation. Selection of distances to consider for exposed population is somewhat arbitrary.

## **2. Ranking the Relative Hazards of Industrial Discharges to POTWs and Surface Waters**

USEPA 1991, Prepared for the Office of Policy Analysis, February 4

The Office of Policy Analysis developed a population weighted hazard index that ranked water bodies and POTWs reported in TRI. OPA used Reportable Quantities as proxies for three risk classes for which ranks were provided. Cancer potency, chronic toxicity, and aquatic toxicity were treated separately in deriving indexes and ranks. For each risk class, each chemical release was divided by the RQ for that risk class. The weighted releases were summed over a selected set such as state or county to arrive at an unadjusted index.

The equation for calculating the unadjusted Hazard Index is:

$$H_i = \sum \frac{R_x}{RQ_x}$$

where:

$$\begin{array}{lll} H_i & = & \text{Hazard Index for set } i \\ R_x & = & \text{Pounds released of chemical } x \\ RQ_x & = & \text{Reportable Quantity for chemical } x \end{array}$$

For each state or county, unadjusted indices were calculated for cancer, chronic, and aquatic toxicity. The indices for cancer potency and chronic toxicity were adjusted using the size of the exposed population to reflect human exposure potential:

$$H_i = \sum \frac{R_x}{RQ_x} \cdot P$$

where:

$$P = \text{Persons per square mile in the county of release } R_x$$

Aquatic toxicity indices were not adjusted using this method due to inadequate data about the size of the exposed aquatic population. Thus, the OPA work does not address the difficult question of adjusting indices based on exposure potential to aquatic life and habitats.

For releases to POTWs, the analysis addressed the hazard of POTW residuals as well as effluent. Average removal rates were applied to chemicals released to POTWs. Standard partitioning rates were applied to the portion removed by the POTW. Hazard indices were then generated for each partitioning pathway (sludge, volatilization) within the POTW.

This methodology was used within the EPA and has not been publicly reviewed.

Pros: Uses peer-reviewed, publicly available toxicity measure (RQs) that are available for a fairly large percentage of TRI chemicals. Also considers county population density as a surrogate measure of exposure potential.

Cons: Does not consider environmental fate of chemicals in exposure evaluation. Use of RQs does not include consideration of severity of effects. RQs do incorporate some consideration of potency, but groupings according to potency are broad.

### **3. Review of Region VII TRI Strategy**

USEPA 1991, Memo from Dermont Bouchard, EPA Region VII to Loren Hall, OTS,  
July 9

Region VII is developing strategies to utilize TRI data. One strategy ranks geographic areas by human health and aquatic ecological risks to determine areas most in need of investigation for further enforcement, remediation, technical assistance, or other purposes. The human health risk analysis, which is separate from the ecological risk analysis, is measured by relative daily toxic loadings (RDTLs). For a given site, an RDTL is estimated for the following categories:

- Non-cancer acute toxicity by ingestion
- Chronic inhalation cancer
- Chronic ingestion cancer
- Chronic inhalation non-cancer
- Chronic ingestion non-cancer

A toxicity measure (for example, the inverse of the RfD for chronic ingestion non-cancer) is multiplied by the site loading to the appropriate media (surface water emission in this case) for each category. These RDTLs are not to be added, unless they are added within a category across the various chemicals present at a site. Because RDTL units are different for each category, they are comparable across sites only within categories.

Aquatic ecological risk for a site is determined in a similar manner. A multi-trophic analysis is used to identify an LC<sub>50</sub> that is the lowest, most protective value for the site. The RDTL is calculated as:

$$RDTL = \text{chemical loading volume} \times LC_{50} / \text{stream volume}$$

Total risk for a site is the sum of the RDTLs across chemicals released at that site.

The Region VII TRI strategy is currently under peer review within the EPA.

Pros: Considers acute and chronic toxic endpoints and multiple exposure pathways. The toxicity measures used (RfDs, q\*, WQC) reflect the relative potencies of chemicals. For ecological risk, more than one trophic level is considered.

Cons: Scores are not combined across sites for a single chemical index; however, scores may be combined within a single site. The human health evaluation categories do not consider environmental fate or population exposure potential. This system is oriented more toward identifying problem sites than in characterizing overall risk from all sites.

### **C. OSWER Scoring and Ranking Systems**

#### **1. Hazard Ranking System; Final Rule**

55 Federal Register No. 241, pp. 51532-51667, December 14, 1990

The Hazard Ranking System (HRS) is the principal mechanism used by the EPA to place sites on the National Priorities List (NPL). It provides a methodology for scoring a site based on various site characteristics. It incorporates information representing four exposure pathways: ground water, surface water, soil and air. If the site's score exceeds an established threshold, the site qualifies for the NPL.

#### **Hazard Ranking Score**

The hazard ranking score is calculated as:

$$HRS = (S_{gw}^2 + S_{sw}^2 + S_s^2 + S_a^2)^{1/2}$$

where:

$S$  = is the scores for each of the four pathways delineated below.

Using the root-mean-square calculation, low migration pathways scores yield a low HRS. However, the HRS score could be relatively high even if only one pathway score was high. This is an important requirement for HRS scoring because some extremely dangerous sites pose threats through only one migration pathway.

While the scoring system for each pathway is quite sophisticated, the pathway scores follow this general methodology:

Likelihood of Release x Quantity of waste at the site x Measure of toxicity x Measure of exposure

The pathway scoring systems demonstrate how toxicity and exposure characteristics can be scored (i.e. weighted). They are much more sophisticated than ordinal scoring systems that implicitly weight characteristics without any underlying justification.

### **Ground Water Migration Pathway**

The pathway score is the product of the following three categories (divided by a scaling factor of 82,500) for the aquifer and contaminant yielding the highest pathway score.

<u>Likelihood of Release</u> x	<u>Waste Characteristics</u> x	<u>Targets</u>
Highest of: Observed release = 550 or Potential to release = Contaminant Score x (Net precipitation score + Depth to aquifer score + Travel time score)	Score of [(Score of Toxicity score and Mobility score) x Weighted Hazardous waste quantity]	Nearest well score + Weighted Population + Resources score + Wellhead score

The scores for these individual components are assigned based on conditions set by the Rule. For example, the contaminant score is 10 if a liner is not present in the containment system, 9 if one is present. The toxicity score is the highest of 1) chronic toxicity score based on ranges for RfDs, 2) carcinogenicity score based on ranges for human carcinogenicity slope factors and weight-of-evidence, and 3) acute toxicity score based on ranges for oral LD<sub>50</sub>, dermal LD<sub>50</sub>, and various LC<sub>50s</sub>. Mobility is scored based on ranges for water solubility and the distribution coefficient (which is based on soil type) of the contaminant. Table 1 of our August 26 memorandum delineates the numerical ranges that compose this scoring method.

The numerous inputs for the groundwater pathway analysis include both chemical- and site-specific measures. Many of these measures are not available for the sites listed on the TRI (for example, chemical waste containment conditions or the characteristics of the geology of surrounding strata.) The following list delineates those measures that are available for many of the TRI chemicals and sites:

Chronic toxicity (human) RfD  
Human carcinogenicity slope factor  
Human carcinogenicity weight-of-evidence  
Oral LD<sub>50</sub>  
Dermal LD<sub>50</sub>  
Dust or mist LC<sub>50</sub>  
Gas or vapor LC<sub>50</sub>  
Water solubility  
Distribution coefficient K<sub>d</sub>  
Quantity or volume of waste  
Population  
Net precipitation  
Depth to the aquifer  
Nearest well

### **Surface Water Migration Pathway**

There are two components for likelihood of release, overland/flood and groundwater to surface water. Each is the higher of an observed or potential release. The component that yields the highest score when multiplied by the sum of the threat scores is the likelihood of release that is used in the HRS score for this pathway. Threats are composed of three categories: drinking water, human food chain, and environmental. The score of each threat is the product of the waste characteristics and targets for that threat.

As with the groundwater migration pathway, surface water migration pathway is based on scoring different conditions regarding site, pathway, environmental, chemical, quantity, and population characteristics. The internal scores are used as weights, not ordinal ranks, for these parameters. The methodology is designed so that worst case conditions determine the final HRS rank. Thus if two exposure routes within a media migration pathway exist for a given site, the most damaging route (as scored) is used to calculate the rank. For example, if the risk of exposure through drinking water is worse than that through fish consumption, the surface water score for the site will be based on risks from drinking water.

The surface water migration pathway scoring system utilizes a combined rating factor to score combinations of toxicity and persistence of a chemical. The factor matrix scores twenty four combinations yielding scores that range eight orders of magnitude.

Like the analysis of the groundwater pathway, the surface water pathway analysis incorporates many measures that are not available for the sites listed on the TRI (for example, the area over which a chemical drains into the surrounding environment.) The following list delineates those measures that are available for many of the TRI chemicals and sites:

Quantity or volume of waste  
Chronic toxicity (human) RfD  
Human carcinogenicity slope factor  
Human carcinogenicity weight-of-evidence  
Oral LD<sub>50</sub>  
Dermal LD<sub>50</sub>  
Dust or mist LC<sub>50</sub>  
Gas or vapor LC<sub>50</sub>  
Half-life in water from combined effects of:  
    hydrolysis  
    biodegradation  
    photolysis  
    volatilization  
Log K<sub>ow</sub>  
Stream volume in cubic feet per second  
BCF  
EPA chronic and acute Ambient Water Quality Criteria  
EPA chronic and acute Ambient Aquatic Life Advisory Concentrations  
Population

### **Air Migration Pathway**

The methodology for this pathway considers gas releases and particulate releases separately. A site which has both kinds of releases is assigned an air pathway score based on whichever kind of release poses the higher risk (as determined by this methodology.) As with the two pathways described above, a release score is based either on an observed release, if present, or on the potential of the site to release. The release score is multiplied by the waste characteristic score and the target score to yield the overall pathway score.

The air water migration pathway methodology is based on scoring different conditions regarding site, pathway, environmental, chemical, quantity, and population characteristics. Specifically, the waste characteristic score comprises measures of toxicity, mobility, and quantity of the chemical released. The target score comprises measures of the nearest individual, surrounding population, natural resources and sensitive environments. Many of the criteria on which scores of these qualities are based are not appropriate for the TRI indicator methodology (e.g. acreage of a nearby sensitive wetland environment.) However, many physical and chemical properties of the chemicals are used as criteria to measure toxicity, mobility, and migration potential. The numerical ranges of these criteria are presented in our August 26 memorandum.

As with the groundwater and surface water migration pathways, internal scores of the air migration pathway are used as weights, not ordinal ranks, in the calculation of the pathway score. In addition, as with the other pathways, the air pathway methodology is designed so that worst case conditions determine the final HRS rank.

Like the analyses of the first two pathways, the air migration pathway analysis incorporates many measures that are not available for the sites listed on the TRI (for example, containment measures in effect and their degree of effectiveness.) The following list delineates those measures that are available for many of the TRI chemicals and sites:

Vapor pressure  
Henry's constant  
Quantity or volume of waste  
Chronic toxicity (human) RfD  
Human carcinogenicity slope factor  
Human carcinogenicity weight-of-evidence  
Oral LD<sub>50</sub>  
Dermal LD<sub>50</sub>  
Dust or mist LC<sub>50</sub>  
Gas or vapor LC<sub>50</sub>  
Population

Note that this ranking system has been published in the Federal Register and has been publicly reviewed.

Pros: A reviewed and published method for evaluating and ranking hazardous waste sites. Evaluates four exposure pathways and adds the scores to yield a single site score. Considers many relevant site and chemical characteristics when scoring exposure. Toxicity score is based on highest of cancer, noncancer and acute toxicity subscores, thereby incorporating consideration of a range of health endpoints. Scores are used as weights, not ranks, so magnitude of exposure and toxicity can be considered.

Cons: Exposure evaluation requires much more detailed site-specific data than are available for TRI sites.

## **2. Application of the Hazard Ranking System to the Prioritization of Organic Compounds Identified at Hazardous Waste Remedial Action Sites**

Hallstedt, P. A., Puskar, M. A., and Levine, S. P (1986) Hazardous Waste and Hazardous Materials, Vol (3):2, pp. 221-232

This system ranks chemicals by relative risk to target those chemicals that are of highest concern with respect to hazardous waste cleanup and the reduction of hazards to human health. The authors' measure of relative risk incorporates the methodology of the first (unrevised) EPA Hazard Ranking System to score chemical toxicity and persistence.

The risk formula that determines the ranking score is straightforward:

$$\text{Score} = \text{Measure of Hazard} \times \text{Exposure}$$

The measure of hazard is based on a chemical's toxicity and persistence characteristics. Each characteristic is ranked from 0 to 3, 3 representing the highest order of toxicity or persistence. The methodologies underlying these rankings are referenced and can be explored if necessary. The overall measure of hazard reflects a synergistic effect between toxicity and persistence and is summarized in the following table:

Measure of Hazard		Persistence			
		0	1	2	3
Toxicity	0	0	0	0	0
	1	3	6	9	12
	2	6	9	12	15
	3	9	12	15	18

Exposure is measured as the percentage of the sample sites that release a chemical weighted by the concentration of each release. Thus, exposure is not an absolute measure of population exposure but a relative measure that is a function of the sample of sites that is used. Concentration of release was used in lieu of volume of release, because data on the latter was unavailable.

Note that this methodology has been published in a peer-reviewed journal.

Pros: Simple, straightforward assignment of chemicals to categories based on toxicity and persistence. Provides relative ranks of chemicals based on toxicity-persistence matrix. Allows for categorization of large number of chemicals, based on available data, SAR, and Best Professional Judgment. Has been published in peer review journal.

Cons: Broad groupings do not permit refined accounting of relative toxicity or persistence of chemicals. Exposure component inappropriate for our purposes, since it considers only the frequency of occurrence of chemicals, and not their concentrations or volumes. Populations exposed are not considered.

#### **D. Office of Water Scoring and Ranking Systems**

##### **1. A Ranking System for Clean Water Act Section 307(a) List of Priority Pollutants**

USEPA 1985, July 3 (Office unknown)

This methodology was developed to determine which chemicals should be added to or subtracted from the Priority Pollutants List, a list of chemicals that pose the greatest hazard to human

health and the environment nationwide in surface water bodies. Chemicals are list candidates if they are either very toxic or exposed to a large population. This system does not attempt to rank chemicals, but simply provides the decision rule for inclusion or exclusion in the list. However, because the chemicals are scored in the process of determining exclusion or inclusion, this system is relevant to the ranking discussion. It is unknown whether this methodology has been peer-reviewed or made available for public comment.

To evaluate toxicity, the following five categories are considered, followed by the variables considered in each category:

- 1) Aquatic Toxicity  
acute ( $LC_{50}$ ), chronic (MATC)
- 2) Mammalian Toxicity  
acute oral ( $LD_{50}$ ), acute dermal ( $LD_{50}$ ), chronic/sub-chronic ( $LDLo$  and  $TDLo$ )
- 3) Human Health  
Evidence of carcinogenicity, mutagenicity and teratogenicity
- 4) Bioaccumulation  
BCF, BAF, Log P
- 5) Environmental Persistence  
environmental half-life, hydrolysis rate, Henry's constant, KD value

Because the variables in a category are often well-correlated, they are considered together to avoid biasing the system by considering the same topic twice. A score is developed for each category by considering the most potent effect of any of the variables in that category. For example, the scoring system for Aquatic Toxicity is:

<u>Score</u>	<u>Acute (<math>LC_{50}</math>) (mg/L)</u>	<u>Chronic (MATC) (mg/L)</u>
12	<0.1	<0.01
10	0.1 to 1.0	0.01 to 0.1
5	1.0 to 10.0	0.1 to 1.0
3	10.0 to 100	1.0 to 10.0
0	>100	>10
*	Insufficient information	

The values of the scores assigned to each category were based on expert judgment. The scoring systems are similar for the other categories. One of the advantages of this method is that data gaps in one variable may be filled by data from another within the same category. Note that in the Human Health category, weight of evidence classes, not numeric measures (such as  $q^*$ ), are assigned score values. If the sum of the scores over the five categories is greater than 10, then the chemical is listed.

National exposure potential is evaluated in a similar manner. The following categories are individually scored on a scale of 0 to 10 based on numerical thresholds as above:

- 1) Amount of discharge nationwide (metric tons per year)
- 2) Number of sites of discharge having detectable concentrations
- 3) Frequency of detection in ambient waters (percent)
- 4) Frequency of detection in aquatic sediments (percent)
- 5) Frequency of detection in industrial or municipal effluents (percent)

If the sum of the scores over the five categories is greater than 10, then the chemical should be listed.

Pros: Considers a range of acute and chronic toxicities. Includes persistence and bioaccumulation. Allows for more than one measure to be used to rank a chemical within one category, thus allowing a wider range of chemicals to be scored. Allows use of expert judgment to fill in data gaps.

Cons: Toxicity ranks are ordinal, not proportional. Since this system was not intended for site-specific use, it is limited in its consideration of exposure potential; exposure potential is based only on environmental fate properties of the chemicals and frequency of occurrence.

## **2. Screening Procedure for Chemicals of Importance to the Office of Water**

USEPA 1986, Prepared by the Office of Health and Environmental Assessment,  
November 14

This screening method was developed by ORD for the Office of Water to differentiate quickly and inexpensively between higher and lower risk chemicals so that the Office could set priorities for more intensive review of a small set of chemicals. Each chemical is identified as having "high", "low" or "unknown" toxicity and "high", "low" or "unknown" exposure. Chemicals are categorized using this matrix:

Rank Categories		Toxicity		
		High	Low	Unknown
Exposure	High	1	2	2
	Low	3	4	4
	Unknown	3	4	4

A fifth and lowest category is reserved for chemicals that are clearly not an environmental problem. Chemicals in this category must either 1) have a half-life of less than a few minutes and not be highly toxic (acute only), 2) be easily treatable, or 3) have not been shown to be toxic at high concentrations.

The criteria for labeling a chemical as having "high" toxicity is different depending on the exposure pathway and exposed population. For example, a chemical exposed to human populations is "highly" toxic if it is a definite, probable or possible carcinogen, or it is developmentally toxic. A chemical exposed to aquatic life populations is "highly" toxic if  $LC_{50} < 100$  mg/l or chronic toxicity  $< 1$  mg/l.

The criteria for labeling a chemical as having "high" exposure is also different depending on the exposure pathway and exposed population. Usually several conditions must be met. Among these, for example, are BCF thresholds and whether or not the chemical has been detected (at any level) in a relevant water pathway.

While "high" criteria are not comparable across pathways and populations, this method succeeds in grouping chemicals roughly by risk. Chemicals not labeled "high" for toxicity or exposure are labeled "low", unless information is unavailable. Data gaps are minimized by using chemical estimation models (ENPART, a fate model; CHEMFATE; CHEMEST.)

It is unknown whether this methodology has undergone peer review or public comment.

Pros: Quick, easy to understand. Assigns rank based on toxicity and exposure potential simultaneously rather than considering these elements separately. Allows scoring of a large number of chemicals based on available data, SAR, and Best Professional Judgment. Considers a range of health endpoints. Implicitly weights cancer and noncancer by automatically assigning "high" ranks to cancer and developmental toxicity.

Cons: Consideration of potency, severity and weight of evidence are implicit, not explicit, in assignment of chemical to one of the toxicity categories. Limited consideration of exposure, based on environmental fate properties and the frequency of detection in U.S. waters.

## **E. Air Office Scoring and Ranking Systems**

### **1. The Source Category Ranking System: Development and Methodology**

USEPA 1990, Prepared for the Office of Air Quality Planning Standards, Chemicals and Petroleum Branch, February 16

This system was devised to rank sources of different emissions in order to prioritize air pollutant source categories. The scoring system looks at both long- and short-term effects of pollutants, taking into consideration pollutant concentrations, maximum and average exposure, the total exposed population, and health risks associated with the exposure. To our knowledge, this system has only been used internally by the EPA and has not been publicly or peer reviewed.

Health effects scores are based upon carcinogenicity, reproductive and developmental toxicity, acute toxicity data, and nonlethal health effects. Before calculating health risk scores, all health

effects are scaled by dividing by the respective maximum health score so that the maximum equals one. Scores for a particular site are then added across pollutants.

Exposure scores were calculated using an algorithm integrated with the Industrial Source Complex Long-Term Model (ISCLT). Exposures per unit loss rates were calculated for both long-term (average) and short-term (peak) chemical releases. These were then scaled by dividing by the maximum exposure score such that the greatest exposure would equal one.

Pros: System was devised to rank air pollutant source categories. It utilizes data on acute and chronic toxicity, pollutant concentrations (as obtained from air modelling), populations exposed and human health risk. Scores are developed for carcinogenicity and other health end points. Scores are summed across pollutants to obtain source specific values. Normalizes scores by dividing each score by maximum value possible in that category.

Cons: System is media-specific to EPA's Air program. The system neither incorporates severity of health effects nor does it allow weight of evidence considerations in scoring. Unknown if system has been peer reviewed. The system also does not include non-human health effects in establishing a source-specific score.

## **2. Measuring Air Quality: The New Pollutants Standards Index**

USEPA 1978, Prepared for the Office of Policy Analysis, July

This index measures air quality based on the potential acute human health effects of five major pollutants: carbon monoxide, photochemical oxidants, nitrogen dioxide, sulfur dioxide, and particulate matter. The index is formed by calculating the following subindex for each pollutant:

$$\text{Subindex} = \frac{100 \times \text{Observed Concentration}}{\text{National Ambient Air Quality Standard (NAAQS)}}$$

The Index value (ranging from 0 to 500) is equal to the highest of the five subindices. The pollutant responsible for the highest subindex and all pollutants with subindices greater than 100 are named (a subindex greater than 100 indicates that the pollutant concentration violates the NAAQS.) Because of the limited definition, indices calculated in this way on a regional or local basis are not comparable because variables such as area of effect, duration of concentration, and exposed population are not controlled.

This index has been published and was designed specifically for public use.

Pros: This index provides a measure of overall air quality based on the potential acute human health effects of five criteria air pollutants. The index is simple and easy to understand. Subindices are calculated for each pollutant by dividing the observed concentration by the relevant National Ambient Air Quality Standard.

Cons: This index is severely limited to just the five criteria air pollutants. The index only incorporates acute health effects data along with ambient air concentration data. It does not look at chronic health effects, ecological effects, populations exposed, weight of evidence considerations, or severity of effects. Additionally, the index does not allow for combining values into a single score.

### **3. National Emissions Standards for Hazardous Air Pollutants for Source Categories: Proposed Regulations Governing Compliance Extensions for Early Reductions of Hazardous Air Pollutants**

USEPA 1991, Prepared for the Office of Air Quality Planning Standards

This proposed rule will implement provisions of the Clean Air Act Amendments of 1990 that allow a source to obtain an extension for compliance with air emissions standards if the source has achieved an overall emission reduction of 90% or more by specified dates. Reductions are calculated based on overall emissions from the source; therefore, a source can use greater than 90% reductions from some pollutants to offset less than 90% reductions for other pollutants to achieve the overall 90% reduction. However, certain rules govern this practice of offsetting for "high-risk" pollutants. Offsetting of these "high-risk" pollutants with lower risk pollutants is calculated based on the relative toxicity of the chemicals. For carcinogens, weighting factors are applied to the emissions of these "high-risk" chemicals, so that every 1 pound of these carcinogens equals between 10 and 1,000,000 pounds of lower risk carcinogens. For noncarcinogens, weighting factors are not developed; rather, chemicals are categorized into two groups, high risk and low risk. High risk noncarcinogens can be traded on a one-to-one basis with other high risk noncarcinogens and with carcinogens on a ten-to-one basis. Reductions in high-risk noncarcinogens can offset low risk noncarcinogens, but not vice versa.

To identify high-risk chemicals in both the carcinogen and noncarcinogen categories, OAQPS first gathered available health data on the chemicals. For carcinogens, potency data was taken from IRIS and from CERCLA Reportable Quantities. Weight-of-evidence classifications and CERCLA hazard ranking (low, medium, high) was also recorded. IRIS was also used to obtain data for noncarcinogens. IRIS was supplemented by RTECS, where IRIS data were not available.

After health data were gathered, OAQPS performed generic exposure modelling based on average meteorologic conditions. If the chemical concentration 500 meters from the source posed greater than  $1 \times 10^{-4}$  risk, or if the concentration exceeded the reference dose (or the LOEL/100 or LD50/1000, if no RfD was available) by an order of magnitude or more, the chemical was preliminarily designated "high-risk". The weighting factors for carcinogens were determined based on the ratio of the potency estimates of the high-risk chemicals to the potency estimates of the lower risk chemicals. In contrast, noncarcinogens were simply placed into high and low risk groups, without specific weighting factors. The last step in the analysis was to determine if any U.S. facilities actually emit these chemicals in sufficient quantities to reach the health effects benchmark of concern. This determination was based on TRI emissions data and other sources of emissions data. If at least one facility released the chemical in sufficient quantities to reach the benchmark exposure level, the

chemical was included on the final "high-risk" list. Note that these emissions standards will be published in the Federal Register.

Pros: The relevant aspect of this proposal is the identification of chemicals that will count toward early emission reduction goals. Importantly, chemicals are ranked as high or low risk using generic air exposure modelling; this would support our use of such a generic approach. Secondly, the system implicitly ranks carcinogens against noncarcinogens by allowing weighted trading among the two types of chemicals. The relative emission trading amounts would support a cancer versus noncancer severity weighting. The approach will be published in the Federal Register.

Cons: System considers only air emissions. System is tailored to a particular requirement of The Clean Air Act Amendments. The system does not address ecological effects.

## **F. Other Agency Scoring and Ranking Systems**

### **1. USEPA Unfinished Business Report: A Comparative Assessment of Environmental Problems**

USEPA 1987, Prepared for the Administrator by  
Richard Morgenstern, Director, Office of Policy Analysis  
Don Clay, Deputy Assistant Administrator for Air and Radiation  
Gerald Emison, Director, Office of Air Quality Planning and Standards  
Rebecca Hanmer, Deputy Assistant, Administrator for Water  
Marcia Williams, Director, Office of Solid Waste  
PB88-127048, February 1987

This EPA report assesses 31 prominent environmental problems currently facing the United States. It attempts to rank them by the risk each poses to society in an effort to prioritize how EPA should use its resources. The environmental problems were defined along existing program lines, e.g. criteria air pollutants, hazardous air pollutants, contaminants in drinking water, Superfund sites, pesticide residues on food, worker exposure to toxic chemicals, etc. The ranking system that the authors employed has been published and peer reviewed by the Scientific Advisory Board.

Four different types of risks were evaluated for each environmental problem: cancer risks, non-cancer health risks, ecological effects, and welfare effects (visible impairment, materials damage, etc.). These risk evaluations did not consider the economic or technical controllability of the risks or the benefits to society of the activities causing the environmental problems. No attempt was made to combine the risk evaluations, so in effect four separate rankings of the 31 problems were generated.

The risk assessments were based on pollutant exposure and effects data. However, because the data were largely incomplete and the methodologies for evaluating them are undeveloped or crude, assessments were ultimately based on the collective informed judgement of the experts involved. Wherever possible, these judgements were made using formal and systematic methods.

### **Cancer Risk**

To assess carcinogenic risk, EPA relied on the Carcinogen Assessment Group's evaluation of the magnitude of risk. However, final rankings were based on judgment of the weight of evidence as well as magnitude.

### **Non-Cancer Health Risk Evaluation**

Each environmental problem was ranked based on the incidence of effects of the chemicals associated with each problem and weighted by the severity of the effects. The methodology began by selecting a few representative chemicals, for which incidence of exposure was estimated:

$$\text{Incidence} = \text{number of people exposed} \times \text{chemical potency}$$

$$(\text{potency} = \text{exposure dose divided by reference dose})$$

Data was often unavailable, in which case the authors' judgement was used. Incidences were summed, weighted by an effect severity index. The final rank was determined by scaling the sum by the authors' estimate of how much of the problem was not captured by the representative chemicals.

### **Ecological Risk**

The authors attempted a broad assessment of environmental impacts on all kinds of ecosystems from terrestrial and freshwater types to marine and estuarine types. However, their assessment was the least rigorous of the four. Each environmental problem was ranked by subjective consensus as high, medium or low for each type of ecosystem. The rankings were based on expert judgement of 1) potential anthropogenic impact on the environment at the local, regional and biospheric levels and, 2) the severity of the impact in terms of number of years required for ecosystem recovery once the stress was removed.

The judgements for a particular environmental problem were systematically aggregated across ecosystems to generate a high, medium or low overall ranking for the problem. However, the authors felt that their method was too inexact to try to establish relative rankings within these categories.

### **Welfare Risk**

A full range of welfare effects were considered, including soiling and other material damages, recreation, natural resources, damages to other public and commercial property and ground water supplies, and losses in aesthetics and non-user values. The environmental problems were ranked by consensus through a subjective review of the extent and cost of existing and potential damage.

Pros: Method is simple. Incorporates four broad risks/effects categories, being cancer risks, non-cancer risks, ecological effects, and welfare effects. These categories allow and require professional

judgment in score determination. The cancer risk score uses both magnitude of risk as well as the weight of evidence. The non-cancer risk score uses exposure as well as severity of effect. This system has been published and reviewed by the Scientific Advisory Board.

Cons: The four different categories cannot be combined into a unified score. The professional judgment went into the score determination rather than the data selection, a process which would prove too unwieldy for the entire TRI database. Both the ecological and welfare ranks were subjective and relied upon site-by-site judgment rather than a rigorous method for calculation.

## **2. Integrated Environment Management Program**

USEPA 1986, Prepared for the Environmental Criteria and Assessment Office, March

The IEMP is one system which seeks to incorporate the severity of the toxicity effect into a chemical release ranking system. The ranking of the chemical release is based upon its relative risk index score, calculated as:

$$RRIS = (Dose) \times (Est. Potency for Human Health Effect) \times (Weighting Factor)$$

Though the algorithm for determining the dose is not specified, the calculation is based upon: (1) pollutant loadings; (2) an exposure analysis using established Agency fate and transport models; (3) the population base identified; and (4) assumptions about body weight and routes of uptake.

Human health effects are divided into eight different categories, i.e. carcinogenicity, mutagenicity, etc. The health score is a function of the probability that the effect occurs in humans (T - based upon a set of decision rules regarding weight of evidence) and the probability of occurrence of the toxic effect (P). For carcinogens, P equals the risk per unit dose. For non-carcinogens,

$$P = I/MED$$

where *I* is the observed incidence of effects above the control incidence at the minimum effective dose (*MED*) expressed as (mg/kg/day).

The weighting factor is actually a severity factor for each toxic effect. They are intended to reflect the significance of the quality of life lost, years of life lost, and economic cost of the disease.

To the best of our knowledge, this system has been used only within the EPA and has not been publicly reviewed.

Pros: Method is simple. It uses both exposure and routes of exposure in its dose calculation. It incorporates eight different health effects in its health score and relies upon the weight of evidence. It can use one or all of these effects, allowing for gaps in the data. It contains a weighting factor for the severity of effect. It also generates a single score for carcinogens and non-carcinogens.

Cons: The system has not, to our knowledge, been peer reviewed. The specifics of the determination of the dose score and health score are not specified in the literature. The allowance of one to all of the health effects in the scoring makes a "fair" comparison among chemicals uncertain.

### **3. Examination of the Severity of Toxic Effects and Recommendation of a Systematic Approach to Rank Adverse Effects**

USEPA 1986, Prepared for the Environmental Criteria and Assessment Office, March

Although this paper did not present a scoring system, it presents information on one aspect of scoring: the weighting of severity among different types of health noncancer effects. Note that it is an internal EPA document and has not undergone public review. The purpose of this paper is to differentiate the effects of chemicals upon the human body and then to rank those effects. For example, two different chemicals may have identical LOELs (Lowest Observable Effect Level) but that the "effects" may be entirely different, i.e. slight changes in the liver versus kidney and/or heart failure. Thus, while current research focusses on comparing chemicals according to these quantities, the author believes in the necessity of a simultaneous ranking system based upon both the type and magnitude of different toxic effects. This paper presents two ranking systems, one for histopathological lesions (direct physical impact upon organs) and one for biochemical effects.

The histopathological scheme lists the severity of effect as a function of the severity of the lesion, modified by any additional non-histopathological effects, and the affected organ. The expression for the severity score is:

$$Score = ((Lesion\ Severity) + (Non-hist.\ Modifier)) \times Organ\ Factor$$

The lesion severity is determined from a table which lists eight possible ranges of effects and then assigns a score from one to eight (eight being the most severe) for that range. The modifier is simply an addend for three different non-histopathological effects: organ weight change, biochemical change, and organ system impairment. For an observed effect in each category, the modifier is one. For no observable effect, the modifier is zero. If it is unknown whether these effects accompany the lesion, the modifier is one-half. A value is assigned to the organ factor according to a table which ranks each of the four "Organ Categories" defined in the report.

The algorithm for the endpoint toxicity scheme is similar. The severity score may be expressed as:

$$Score = ((Endpoint\ Severity) + (Endpoint\ Modifier)) \times Organ\ Factor$$

The endpoint severity is determined from a table which lists seven possible ranges for the biochemical change or system impairment as well as the category of the affected organ. The table assigns a score, from one to seven, for each range, with seven being the most severe. The modifier, as in the first scheme, is equal to one, zero, or one-half, depending upon an observed, non-observed, or uncertain accompanying histopathological lesion or organ weight change. For example, a body

weight change in an organism receives a score of one, the absence of organ weight change and lesions creates a modifier of zero for both and therefore a total modifier of zero. No effect in category one organs (lung, heart, brain, etc.) is an organ factor of one, yielding a total score of one.

The author cautions that these proposed schemes are not suitable for use in the comparison of chemicals because, since factors such as duration of exposure and route of exposure were not variables in the derivation of the schemes, these would need to be held as fixed in comparing chemicals, a situation which never occurs in toxic releases.

Pros: A relatively simple method. It examines the differences in the severity of effects. It includes rankings according to the organs affected, biochemical effects, and histopathological effects.

Cons: This is not an overall scoring system. The author even cautions against its integration into a scoring system because certain site-specific variables, such as duration or route of exposure, were not incorporated into the scheme. This system has not been peer reviewed.

In developing this severity ranking scheme, the authors of this paper reviewed several other systems that use severity as a factor in the comparison of chemicals. The following describes systems used by the author to develop their scoring systems.

#### **Assessment of Air Emissions from Hazardous Waste Treatment, Storage, and Disposal Facilities**

One hundred of the 501 RCRA wastes handled by treatment, storage, and disposal facilities (TSDFs) were ranked according to two types of health data, toxic effects and carcinogenic effects. Two factors were created, the toxicity hazard factor and the carcinogenicity hazard factor. These are described as:

$$THF = (gas-phase equil. conc.) / (Threshold Limit Value)$$

$$CHF = (gas-phase equil. conc.) / (max allow. conc. at the 1E-5 Risk Level)$$

The maximum allowable concentration at the 100,000 risk level is the concentration at which there is a 95% confidence that the limit on the cancer risk is one in one hundred thousand people. Each of these factors is then multiplied by the wastes' aqueous and nonaqueous disposal volumes in order to generate volume-weighted hazard scores.

In addition to the determination of these factors, a weighting factor is created from carcinogenicity, teratogenicity, and acute toxic effects of each contaminant (using data from RTECS). The score for each lies between zero and three. This weighting factor was then multiplied by the scores.

Pros: Simple system. Incorporates two different health effects, toxic effects and carcinogenic effects. It uses the volume of release directly in the score determination. Includes a weighting factor based upon carcinogenicity, teratogenicity, and acute toxic effects.

Cons: The two scoring factors for toxic and carcinogenic effects cannot be combined. The factors rely upon the Threshold Limit Value and the Maximum Allowable Concentration at the 1E-5 Risk Level respectively, data which exists for few chemicals. Does not have an exposure component.

### **RCRA Risk-Cost Analysis Model**

This model follows a five-step process in order to determine human health risks resulting from releases of chemicals. After chemical selection, concentrations of the contaminants are estimated for three transport processes (air, surface water, and groundwater). The model then estimates the total human intake, calculates the risk to an individual, and then estimates the population risk by multiplying by the total population in a given area. This process assigns a risk score which then ranks the releases.

Two equations were developed in order to model the process. They are:

$$\text{Carc. Risk} = (\text{risk per unit dose}) \times (\text{severity index}) \times (\text{dose})^{\text{shape}} \times (\text{population exposed})$$

$$\text{Non-Carc. Risk} = (\text{risk per unit dose}) \times (\text{dose}) \times (\text{population exposed})$$

The severity index follows from a 1984 EPA ranking system developed to quantify statutory reportable quantities of hazardous substances. It assigns a value of 0.1 for severities 1-2, 0.5 for 3-7, and 1.0 for 8-10. The shape is merely an exponent to determine the shape of the curve.

Pros: Simple System, requiring only a dose for mammalian species based upon either human or animal chronic or acute doses. Considers three different routes of exposure, oral, inhalation, and dermal.

Cons: Relies upon a narrow range of health effects. Does not have an exposure or a volume component (it ranks chemicals, not releases). Though the score only requires the dose, the calculation of the dose is a cumbersome and difficult to understand process.

### **Toxicity Scoring System Using RTECS Data Bases**

Though the scoring algorithm is simple, requiring only a dose, the methodology requires detailed toxicity data for input into the algorithm.

The only dose considered are those for mammalian species. This method only considers oral, inhalation and dermal routes of exposure, assuming each of equal importance and the absorption to

be 100%. Four subscores are considered for each substance: human acute, animal acute, human chronic, and animal chronic. The final score is taken from the following hierarchy:

- ! minimum of human and animal chronic doses, if both have entries;
- ! chronic dose for humans or animals, if only one has entry;
- ! minimum of human and animal acute doses, if both have an entry and there are no chronic entries; and
- ! acute dose for humans or animals, if this is the only category with any entries

In using RTECS, chronic exposures are those resulting in effects other than death or are effects such as cancer which may result in mortality. Selecting a human chronic effect requires comparison in the RTECS data bases, where carcinogenic effects are classified as a carcinogenic response (CAR), a neoplastic response (NEO), or an equivocal tumorigenic agent (ETA). The lowest effect level for carcinogenicity is chosen by selecting the lowest dose of CAR or NEO. If neither exists, the lowest ETA is multiplied by two. The selected dose is modified when there are multiple carcinogenicity entries by decreasing the selected dose 10 percent per additional positive result, to a maximum of 50%. Teratogenic doses from individual studies are ranked and the dose at the 20th percentile is selected as the teratogenic dose. This dose is lowered in the same manner as the carcinogenic dose.

Pros: Simple system. Incorporates exposure data for three different routes, air, surface water, and groundwater. It also incorporates the severity of effect according to a 1984 EPA ranking system, making its inclusion simple and straightforward.

Cons: Relies strictly upon the cancer slope of a chemical, limiting the number of allowable chemicals by available data. The two separate scores calculated, carcinogenic and non-carcinogenic, may not be compared.

## II. Survey of TRI Ranking and Indexing Efforts Outside EPA

A number of organizations outside of the Agency have also developed ranking/scoring systems for their own purposes, such as targeting chemicals for state regulation; identifying chemicals for pollution prevention projects; and assessing the hazard of TRI emissions in particular communities.

Abt Associates contacted a number of organizations which have utilized TRI data in publications. The organizations were asked about the scope and methodology used in their reports.

**Rhone-Poulenc** in Paris developed an Environmental Index (EI) to assess the aqueous effluent impact of wastes. They computed a raw indicator as a weighted average of the daily mass of six types of wastes (toxic materials, suspended solids, nitrogen, phosphorus, salts, and chemical organics). No justification is given for these weights. The raw indicator is multiplied by 100 and divided by the average from the prior year to arrive at the final EI for the month. This transformation

is intended to make comparisons easy. If the index is greater than 100 the impact has been greater, values less than 100 indicate improvement.  
(Rhône-Poulenc memo July 25, 1991)

**Chemicals on Which Data Are Currently Inadequate: Selection Criteria for Health and Environmental Purposes**

Organization for Economic Co-operation and Development, Berlin, March 1985

This report itself did not present a chemical ranking system. Rather, the purpose of this task was to develop a rational methodology by which countries could select chemicals that most urgently need attention. The elements of this methodology were: identifying selection elements, exploring ways of weighting and combining elements and reviewing data sources. Selection elements identified included workplace exposure, general population exposure, environmental exposure, human and environmental effects. OECD also included recommendations for applying these elements. Importantly, OECD emphasized the importance of clarifying the purpose and scope of the selection exercise in order to define limits and interpretations. OECD also supported the use of expert judgment to fill in data gaps. Finally, OECD strongly urged consideration of data quality in the ranking and selection of chemicals.

For each of the elements of the methodology, OECD broke the approach down into four steps: compilation, screening, refinement and review. The report then suggested topics to consider in each of the four phases.

**Polaroid Corporation** has developed a 5-category scheme for all chemicals that they use. Chemicals in categories i and ii are highly toxic (known and possible carcinogens). Category V chemicals are non-toxic solid waste. Chemical categories have been used to establish goals for 50 percent reduction in chemical use by category. The focus on chemical use reduction rather than chemical release reduction is based on the Massachusetts Toxics Use Reduction Act. Category specific goals are designed to prevent strategies that claim a "50 percent use reduction" but are based exclusively on reductions in use of low toxicity wastes.

(Conversation with Polaroid Corporation representatives, June 1991)

**The Boston Herald** published a series of articles under the heading of "Ill wind," covering environmental releases of toxic chemicals in Massachusetts. The Herald concentrated mostly upon volumetric data but also developed an algorithm for ranking the chemical releases according to volume and toxicity. The algorithm multiplied the volume of release by a decimal number derived from the inhalation risk number. This enabled the article to rank individual emitters by order of "cancer risk." The Herald acknowledged that the ranking did not incorporate human exposure into its calculation and cautioned against using their calculation as an "actual measurement of risk"  
(The Boston Herald, Monday, May 13, 1991, p. 8).

## **Air Toxic "Hot Spots" Program Risk Assessment Guidelines**

California Air Pollution Control Officers Association, March 1990

This system is designed to prioritize facilities in accordance with the Air Toxics "Hot Spots" Information and Assessment Act of 1987. According to this act, any facility which qualifies as a "high priority" facility must perform a health risk assessment. Localities determine the priority level (high, intermediate, or low) of the facilities in their district based upon the facility's reported emissions of one or more of some 500 chemicals. Separate calculations and priority levels are used for carcinogenic and noncarcinogenic substances. The higher of the two levels as calculated is assigned to the facility.

The score for a facility emitting carcinogens is equal to the sum of the scores generated for each carcinogen. Each contaminant's score is calculated as

$$TS = \text{emissions [lbs/yr]} \times \text{unit risk } [\mu\text{g}/\text{m}^3]^{-1} \times \text{distance factor} \times \text{normalization factor}$$

The distance factor is determined from the distance from the source of the emissions to the nearest populated area. That quantity corresponds to a value relating the change in concentration with distance through the use of a Gaussian plume dispersion model. A total score of ten roughly corresponds to a risk of one in ten thousand and a total score of one similarly corresponds to a risk of one in one hundred thousand. This methodology places any facility scoring above ten in the "high priority" category and those scoring below one in the "low priority" category. A score between one and ten requires further analysis.

The score for a facility emitting non-carcinogens is determined much in the same way. The total score for the facility is the sum of the scores of each substance emitted by the facility. The substance score may be expressed as:

$$TS = \text{emissions [lbs/yr]}^{16} \times \text{distance factor} \times \text{normalization/acceptable exposure level } [\mu\text{g}/\text{m}^3]$$

The non-carcinogenic scores are considered identically to the carcinogenic scores, with "high priority" assignment to facilities with totals over ten and "low priority" assignment to facilities with total scores below one. Note that the carcinogenic and non-carcinogenic scores are not added together.

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<sup>16</sup>maximum lbs/yr for substances associated with acute toxicity and average lbs/yr for substances associated with chronic toxicity

## **Louisiana's Environmental Action Plan "Leap to 2000"**

Public Advisory and Steering Committee Risk Ranking Retreat Briefing Material

March 26, 1991

Louisiana formed a Political Advisory Committee (PAC) to rank 33 environmental issues by the severity of risks they posed to the State. Risks were divided into three categories, human health, ecological effects, and quality of life. The issues were ranked separately within each of these categories based upon available scientific information and the judgement of assembled experts. Informed by the three rankings, the PAC settled the final comprehensive risk ranking by voting on the issues.

### **Health Effects**

This method estimates risk to human health from the cancer and non-cancer effects. Cancer risk was calculated based on chemicals representative of each issue:

$$\text{Risk} = \text{Environmental Concentration} \times \text{Potency} \times \text{Population Exposed}$$

Thus the issues were ranked by estimated cancer cases that would be caused by a particular environmental problem. The issues were categorized as high, medium or low based on breaks in the data of these results.

Non-cancer health risk was estimated from chemicals representative of each issue. Three exposure pathways were considered: air inhalation, food and liquid ingestion, and skin adsorption. Risk presented by each issue was calculated for each applicable exposure scenario as:

$$\text{Risk} = \text{Severity Index} \times \text{Dose} \times \text{Population Score}$$

The severity index is a standard ordinal ranking of body organs affected by a chemical and the severity of those affects. Dose is an ordinal score based on ranges of RfD divided by average contaminant concentration in the population's environment. Population score is an ordinal rank of ranges of population sizes.

Non-cancer health risk for an issue is calculated as the average of the risks posed by each exposure pathway. Issues were again ranked high, medium or low based on breaks in the data of these results.

The final issue ranking placed equal weight on the cancer and non-cancer effects. The nine possible combinations of the elements of the two categories were assigned very high, high, medium high, medium and low ranks based on a committee consensus.

### **Ecological Effects**

The ranking committee ranked the environmental issues based on the degree to which nine ecosystems were affected by each issue. Impacts on each of the nine ecosystems were evaluated on an issue by issue basis by examining how stressors associated with an issue impacted the stress indicators in an ecosystem. For example, for the Terrestrial Habitat Loss issue, stressors like industrial development and proposed road construction were rated on a scale of 0 to 10 for how they affect such stress indicators as Changes in Nutrient Cycling and Loss of Habitat. A stressor's score was the weighted average of ratings across stress indicators, the weights reflecting the committee's assessment of relative importance of the stress indicators. Stressor scores were averaged to determine the final rating of the importance of the issue to the particular ecosystem.

The rank of the issue was calculated as the weighted average of these ecosystem-specific ratings, the weights reflecting the committee's assessment of the value of each ecosystem. Breaks in the ranking figures determined how the issues were divided into five categories (very high through low.) Separately, committee members voted on the ecological importance of each issue using the same five categories and compared this ranking to the quantitative one. The four issues that were not placed in the same categories by the two systems were recategorized by consensus.

### **Quality of Life**

This analysis attempted to rank the issues into high, medium and low categories based on the costs associated with damages not accounted for in the two other rankings. Among these costs are health care costs, recreation losses, materials damage and aesthetic losses. The issues were first ranked based on the dollar value estimates of costs as determined by various relevant economic studies. The issues were ranked again based on qualitative assessments of changes in quality of life using such measures as the number of people suffering damages, and the reversibility of those damages. Equal weight was given to the quantitative and qualitative rankings in determining the final ranking (again using the very high through low categories.)

### **Purposes of and Criteria for Development of Chemical Hazard Lists from Ten Domestic and International Organizations**

USEPA 1985, Prepared for the Office of Pesticides and Toxic Substances, Economics and Technology Division, December 31

This report reviewed various systems by which different organizations have compiled lists of chemicals which they believe ought to be monitored. Each of these steps involved selecting criteria in order to determine their placement upon the list as well as ranges. The following summarizes the findings of this report:

**The European Communities Council Directive Chemical Hazard List:**

82/501/EEC, OJ No L 230, 5.3.82, pp. 1-18 (June 24, 1982)

The EC has mandated that any industry must list their use of any of the 178 chemicals upon this list. The chemicals on this list fall into two toxic categories, very toxic substances, other toxic substances. The qualifications for these categories are as follows:

"Very Toxic" Substances	Other Toxic Substances
$LD_{50}$ (oral) $\leq 5$ ; or $LD_{50}$ (cutaneous) $\leq 10$ ; or $LC_{50}$ (inhalation) $\leq 0.1$  or $5 < LD_{50}$ (oral) $\leq 25$ ; or $10 < LD_{50}$ (cutaneous) $\leq 50$ ; or $0.1 < LC_{50}$ (inhalation) $\leq 0.1$ and Physical and chemical properties which cause effects similar to those caused by chemicals which fall into the above criteria	$25 < LD_{50}$ (oral) $\leq 200$ ; or $50 < LD_{50}$ (cutaneous) $\leq 400$ ; or $0.5 < LC_{50}$ (inhalation) $\leq 2$

**California Air Resource Board Toxic Chemical List & NIOSH/OSHA Pocket Guide:**  
Air Resources Board of the State of California

The NIOSH/OSHA Pocket Guide to Chemical Hazards is a list of 380 chemicals, all under federal regulation, which includes information on and recommendations concerning each of these chemicals. The object of this list is to compile chemicals most likely to travel downwind in the event of an accidental release. The California Air Resources Board included on its list any chemical from the guide with an IDLH (Immediately Dangerous to Life and Health - maximum concentration of a substance from which one could escape within 30 minutes without any escape-impairing symptoms or any irreversible health effects) below 2000 ppm and a vapor pressure greater than 20 mmHg.

**New Jersey Department of Environmental Protection Highly Toxic Substances List:**  
State of New Jersey Department of Environmental Protection, Division of Environmental Quality

The division of Environmental Quality in the Department of Environmental Protection in New Jersey sought to prepare a list of chemicals which would cause acute health effects if released into the air. Their toxicity criterion was based upon a Threshold Limit Value (TLV - time-weighted average concentration to which nearly all workers may be repeatedly exposed without adverse effect) of one pm. An additional criterion for inclusion on the list was reactivity. Volatility and usage were used to rank the chemicals, but the methodology is not included in the report.

**Department of Transportation Poisonous Substances List:**  
DOT Hazardous Materials Regulations 49 CFR 172.101

The DOT's Hazardous Materials Table includes two categories for poisonous substances, Poison A and Poison B. Poison B materials meet the following requirements:

$$LD_{50}(oral) \leq 50 \text{ mg/kg}$$

$$LC_{50} (inhalation) \leq 2 \text{ mg/l (if such a conc. is likely)}$$

$$LD_{50} (cutaneous) \leq 200 \text{ mg/kg}$$

The Poison List has 153 chemicals of which 141 are Poison B materials.

**Philadelphia Air Pollution Control Board Toxic Air Contaminants List:**

Air Management Regulation VI: Control of Emissions of Toxic Air Contaminants, Air Pollution Control Board of the Philadelphia Department of Public Health, 1981

Two lists were developed in order to require emissions reports from industry. The criteria for the development of Schedule A are not specified, though the methodology incorporated risk of immediate harm, carcinogenicity, mutagenicity, teratogenicity, bioaccumulative effects, and whether the chemical is known to be present in the Philadelphia area. The criteria for schedule B are identical and also meet the definition of "pollutant" as established by the EPA. The two schedules encompass a total of 104 chemicals.

**Union Carbide Corp. Industrial Hygiene Sampling and Monitoring Program List**

Union Carbide Institute plant, 1984

Union Carbide developed a list of priority chemicals for their monitoring program at their plant in Institute, West Virginia. The chemicals have been ranked ordinally from one to four in the following system:

Rating 4	Rating 3	Rating 2	Rating 1
<p>Have OSHA, ACGIH, or UCC standards (whichever is lower) including permissible exposure limits (PEL) of less than 5 pm or less than 0.1 mg/m<sup>3</sup> as TWA<sub>8</sub> (time weighted average for normal 8 hr. day)</p> <p>known carcinogens</p> <p>result in mutagenesis, teratogenesis, or fertility impairment in humans</p> <p>result in irreversible nerve damage</p> <p>result in irreversible long-term organ toxicity</p> <p>are fast-acting and can produce major injury</p>	<p>5&lt;PEL&lt;25 or .11&lt;TWA<sub>8</sub>&lt;1.0</p> <p>supposed human carcinogens, mutagens and teratogens</p> <p>result in hematologic disturbances</p> <p>result in respiratory of skin sensitization</p> <p>produce narcosis</p>	<p>26&lt;PEL&lt;200 or 1.1&lt;TWA<sub>8</sub>&lt;5</p> <p>produce severe irritation of the skin, eyes, or respiratory system</p> <p>are anoxiants</p>	<p>PEL&gt;200 or TWA<sub>8</sub>&gt;5</p> <p>classified as simple asphyxiants or nuisances</p> <p>have generally low risk effects</p>

The ranking of the chemical determines how often they are to be sampled within the plant.

As can be noted, each of these systems represents a methodology for chemical selection and presents, at best, a simplistic means for ranking chemicals according to different properties. Nonetheless, it presents a large sample of properties (PEL, IDLH, etc.) which have been used in the differentiation of chemical toxicity.

### **Other Systems**

Our research has uncovered three systems for which we are still trying to obtain documentation. They are an Office of Water TRI chemical ranking system, an EPA compound evaluation system, and the National Air Toxics Information Clearinghouse pollutant selection and prioritization method. We also found two systems that were not relevant to this TRI indicator discussion. The documents supporting these systems are titled 1) Existing Chemicals of Environmental Relevance (German Chemical Society, October 1985) and 2) Chemical Scoring System Development (Oak Ridge National Laboratory.)

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## **Appendix B**

### **Options for a TRI Indicator Ranking/Scoring System**

## Appendix B

### OPTIONS FOR A TRI INDICATOR RANKING/SCORING SYSTEM

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## **I. Elements of a Scoring System**

Appendix A summarizes a number of chemical scoring and ranking procedures used by Offices within the Agency and by organizations outside of the Agency. From the review of these scoring systems, several common issues emerge. These issues must be considered for the development of a ranking system for the TRI Indicator. These issues include:

- a. Selecting measures on which the ranking will be based  
Choosing measures to describe a chemical's toxicity and potential exposure
- b. Selecting a method to score the measures. Options include:  
Qualitative - high, medium or low  
Ordinal - 1, 2, 3  
Weighted Categories - 10, 100, 1,000  
Calculated - continuous values
- c. Defining criteria for weighted categories  
For example, an chemical may be scored a 1 if its RfD falls between 0.5 to 5 and a 10 if its RfD falls between 0.05 and 0.5  
Weight-of-evidence categories might also be scored
- d. Factoring data quality into the indicator
- e. Using severity of effect to weight chemical scores
- f. Ranking individual chemicals or forming sub-indices  
Each chemical can cause a range of effects (e.g. acute toxicity, neurotoxicity, cancer). If the relative importance of effects is established, a chemical can be scored on each type of effect that it causes, then its scores can be combined across effect categories to form a single score for that chemical. If the relative importance of risks cannot be established, a separate indicator for each type of toxicity can be generated, or the weight can be based on the most sensitive effect caused by the chemical.
- g. Methods of establishing the relative importance of categories  
If different categories are used, the relative importance can be reflected by the methodology used to combine the category scores. Various methods include simple summation, multiplication, other mathematical functions, matrices, taking the worst score, and establishing decision rules
- h. Weighting scores: an alternative to methods presented in Section I.g.

The review of the scoring systems within and outside of the Agency has suggested a number of approaches for handling each of these issues. Several alternative approaches for each issue, and their advantages and disadvantages, are described below.

#### **A. SELECTING MEASURES ON WHICH THE RANKING WILL BE BASED**

Measures upon which to base scoring include those that describe the toxicity and physicochemical properties of a chemical (e.g., LD<sub>50</sub>, RfD, solubility), and others that describe exposure at a site (e.g., volume of release, population, site environments). The Section 313 criteria lists ten parameters that EPA must consider when evaluating a chemical for addition to TRI: carcinogenicity, chronic toxicity, acute toxicity, reproductive toxicity, heritable gene and chromosomal mutations, developmental toxicity, neurotoxicity, environmental toxicity, persistence and bioaccumulation. Most of the scoring systems reviewed consider at least some of these categories, although they are frequently merged into fewer parameters.

The indicator could also incorporate measures of potential exposure including media-specific emissions volumes, site characteristics and physicochemical properties. Site characteristics include the potential population exposed through different media, and factors such as stream volume and wind speed that influence the transport and dispersion of a chemical in the environment. Physicochemical properties typically include partitioning, dilution, and dispersion coefficients of contaminants.

#### **B. SELECTING A METHOD TO SCORE THE MEASURES**

A system for evaluating the measures of toxicity and exposure potential must be chosen. The goal is to derive some way of scoring chemicals relative to one another within each category. Possible categories might be human carcinogenicity, human chronic toxicity, mammalian acute toxicity, chronic toxicity for aquatic species, and physicochemical exposure potential.

One possible system uses qualitative divisions to score chemicals within a category. For example, the carcinogenicity of a chemical might be scored "high", "medium", or "low." An advantage to using qualitative scores is that a broad range of information, qualitative and quantitative, can be used to evaluate chemicals; this would allow assignment of scores to chemicals without specific toxicity or exposure data. A disadvantage of qualitative scores is that they only broadly distinguish toxicity and exposure potentials and limit the usefulness of the Indicator as a priority-setting system. Ordinal systems (e.g. 1, 2, or 3) use numbers rather than "low," "medium" or "high" to rank chemicals. Note that ranking formulas that incorporate ordinal scores should not be used to attribute proportional meaning to the ordinal scores. Because assigning an ordinal rank of 3 to chemical A and 1 to chemical B does not mean chemical A is three times worse than chemical B, mathematical functions involving these two scores only convey information on order, not on proportional magnitude.

Unlike ordinal systems, that simply rank relative attributes of chemicals, order-of-magnitude scoring systems (e.g. 1, 10, 100, 1000) still use numerical scores, but attempt to incorporate more information about the proportional differences between chemicals. For example, proportional scores for toxicity could reflect the proportional magnitudes of cancer potencies among chemicals. Weighting chemicals using proportional categories of toxicity uses more information about the chemicals but also avoids the impression of accuracy where such accuracy does not exist. Also, defining categories of weights allows EPA analysts to use all relevant toxicity information about chemicals to make approximate judgments about relative order of magnitude of toxicity, even for chemicals where specific slope factors and RfD values have not yet been developed by the Agency, thus allowing more chemicals to be included in the Indicator. Finally, chemicals are likely to remain in the order-of-magnitude toxicity category to which they are originally assigned, unless significant new and different toxicity data become available. Thus, the weights applied to these chemicals are not likely to be revised frequently, lending stability to the Indicators over time.

Another way to score chemicals within a category is to use an actual numerical value of a measure or mathematical function of the measure. For example, carcinogenicity might be scored by using the actual slope factor of each chemical. Such a system compares chemicals on a continuous scale and allows for the greatest use of quantitative data and results in the greatest distinction among chemicals. However, continuous weights based upon specific information (based on  $q_1^*$  or on chemical-specific decay rates, for example) have some disadvantages. First, continuous weights would imply that we know the toxicity of the chemical with enough accuracy to distinguish among relatively small differences in these values. In fact, there are significant uncertainties associated with the assessment of a chemical's slope factor and even weight-of-evidence. In fact, the definition of the RfD contains the expression "within an order of magnitude." Second, it would limit the number of chemicals in the Indicator to those for which the specific information is available, and limits the use of qualitative information and professional judgment.

### C. SELECTING RANGES OVER WHICH MEASURES ARE ASSIGNED SCORES

If a proportional, order-of-magnitude system is used to rank chemicals, then the categories must be assigned to a range of values of the underlying measure. For example, the 307(a) Priority Pollutants Chemical Ranking methodology used the following ranges to score the aquatic toxicity of chemicals:

<u>Score</u>	<u>LC<sub>50</sub> (mg/L)</u>
12	< 0.1
10	0.1 - 1.0
5	1.0 - 10.0
3	10.0 - 100
0	> 100

The categories can be defined using ranges of a number of types of data; for toxicity weights, for example, RfDs (non-carcinogens) and  $q_1^*$  (carcinogens), RQs (or TPQs where RQs not available), and occupational levels could be used.<sup>1</sup> The selection of ranges forces a tradeoff between 1) using a large number of narrow ranges, which might imply that the data is more refined than it really is, and 2) using a small number of broad ranges which inflates or diminishes the importance of the boundaries and the measures that fall near them.

More than one kind of measure can be used to score chemicals within a category. This approach takes advantage of a broader data set to score chemicals, including structure activity relationships. For example, for acute mammalian toxicity, we may have several kinds of toxicity data that describe a chemical's potency, such as acute oral LD<sub>50</sub> and acute dermal LD<sub>50</sub>. If only one measure were available, it would be used to determine the chemical's rank in that category. If both were available, the more restrictive value could be used. Alternatively, a hierarchy of preferred measures could be established; for example, RfDs may be preferred over RQs. The advantage is that a larger number of chemicals can be assigned a weight.

The selection measures, boundaries for scoring measure ranges, and category scores are presented in Tables 1, 2, 3 and 4 for selected scoring systems reviewed. The review demonstrates that vast effort and expertise has already been devoted to scoring and categorizing chemicals, both within the Agency and externally. This expertise could be built upon in the development of the TRI Indicator.

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<sup>1</sup>Edward J. Calabrese and Elaina M. Kenyon, "The Perils of State Air Toxic Programs," *Environmental Science and Technology*, Vol. 23, No. 11 (November 1989), 1326-9. This article warns against using occupational levels for general population risk screening, for several reasons: (a) occupational levels consider a recovery period between exposures; (b) occupational levels consider the "healthy worker" effect (that is, the levels are set for protection of relatively healthy populations), (c) the ACGIH levels are set based on data of unknown quality (d) the levels do not account for environmental fate (persistence, bioconcentration) and multiple exposure sources.

Table 1: Human Toxicity Parameter Ranges

Ranking Systems	Human Acute Toxicity			Human Chronic Toxicity			
Screening Methodology for Pollution Prevention Targeting (USEPA, date unknown, prepared for Office of Toxic Substances)				Carcinogenicity: high = 3 med = 2 low = 1  all B2 carc. given a score of 3	Neuro: high = 3 med = 2 low = 1	Developmental: high = 3 med = 2 low = 1	
Ranking the Relative Hazards of Industrial Discharges to POTWs and Surface Waters (USEPA 1991, prepared for the OPA, February)				Carcinogenicity: Cancer RQ Value Used Directly	Non-cancer chronic: Chronic RQ Value Used Directly		
Hazard Ranking System; Final Rule (55 Federal Register No. 241, pp.51532-667, 12/14/90)	LD50 (oral) < 5 mg/kg 5-50 50-500 > 500 not available	LD50 (dermal) < 2 mg/kg 2-20 20-200 > 200 not available	Ranking: 1,000 100 10 1 0	Carcinogenicity: Class A, Slope Factor 0.5 < 0.05-0.5 < 0.05 - not available	Class B, Slope Factor 5 < 0.5-5 0.05-0.5 < 0.05 not available	Class C, Slope Factor 50 < 5-50 0.5-5 < 0.5 not available	Ranking: 10,000 1,000 100 10 0

Ranking Systems	Human Acute Toxicity			Human Chronic Toxicity	
Hazard Ranking System; Final Rule (55 Federal Register No. 241, pp.51532-667, 12/14/90) (concluded)	LC50	LC50	Ranking:	Non-cancer chronic:	
	(dust or mist)	(gas or vapor)		RfD	Ranking:
				<0.0005 mg/kg/day	
	< 0.2 mg/l	< 20 mg/l		0.0005-0.005	10,000
	0.2-2	20-200		0.005-0.05	1,000
	2-20	200-2,000		0.05-0.5	100
	> 20	> 2,000		0.5 <	10
USEPA Unfinished Business Report	not available	not available	0	not available	1
					0
				Dose/RfD	Score
				1-10	1
				10-100	2
"Hot Spots" Program				100-1,000	3
				> 1,000	4
				Air:	
				Carcinogenicity:	Non-cancer chronic:
				q*	RfD
				Used	Used
				Directly	Directly

Ranking Systems	Human Acute Toxicity			Human Chronic Toxicity
Land Disposal Branch Office of Solid Waste				Threshold Limit Value (TLV)  Used Directly  (Concentration Units)
European Communities Council Directive Chemical Hazard List	LD50  (oral)  "very toxic"  <= 25  "other toxic"  25-200	LD50  (cutaneous)  "very toxic"  <= 50  "other toxic"  50-400	LC50  (inhalation)  "very toxic"  <= 0.5  "other toxic"  0.5-2	
A Ranking System for Clean Water Act Section 307(a) List of Priority Pollutants (USEPA 1985, July)				Score    Carcinogenicity: 12    Proven human carcinogen 10    Potential human carcinogen, proven animal carcinogen 5    Potential animal carcinogen, proven mutagen, proven teratogen 2    Potential mutagen, potential teratogen 0    No carcinogenic, mutagenic, or teratogenic properties

Ranking Systems	Human Acute Toxicity					Human Chronic Toxicity	
TSCA Chemical Scoring System for Hazard and Exposure Identification	Inhalation	Dermal	Oral	Exposure		Score	Genotoxicity:
	LC50	LD50	LD50	Level	Score	9	Evidence of mammalian mutagenicity/clastogenicity, interaction with mammalian germ cell DNA, or epidemiological data suggesting genotoxicity in humans
	< 50 mg/m3	< 200 mg/kg	< 50 mg/kg	Low	7-9		
	50-500	200-500	50-500	Medium	4-6	8	Evidence of genotoxicity in non-mammalian germ cell assays, or evidence of mammalian dominant lethality
	> 500	> 500	> 500	High	1-3	5-7	Evidence of genotoxicity in more than one test system, other than above
						2-4	Limited evidence of genotoxicity, including mixed positive and negative results
						1	Limited evidence of nongenotoxicity
						0	Negative test results indicating lack of known genotoxicity
						Score	Carcinogenicity:
						8-9	Evidence of oncogenicity from epidemiological studies or positive results in two or more mammalian species
						6-7	Evidence of oncogenicity in either sex of a single mammalian species
						4-5	Suggestive evidence of oncogenic potential from epidemiological studies, mammalian bioassays, cell transformation in vitro, or promoter/carcinogenic activity
						3	Evidence of genotoxic potential
						1-2	Limited evidence of lack of oncogenic potential
						0	No evidence of oncogenic potential from well-conducted and well-designed mammalian studies in two or more animal species

Ranking Systems	Human Acute Toxicity		Human Chronic Toxicity			
TSCA Chemical Scoring System for Hazard and Exposure Identification (continued)			Score	Developmental Effects:		
			8-9	Evidence of adverse developmental effects in humans or at least two other mammalian species		
			6-7	Evidence of adverse developmental effects in one mammalian species		
			5	Developmental effects at doses accompanied by maternal toxicity or otherwise equivocal test results		
			4	Adverse developmental effects in nonmammalian species or in vitro test systems		
			3	Indirect evidence suggesting possible adverse developmental effects		
			2	Indirect evidence of lack of adverse developmental effects		
			1	Limited evidence of lack of developmental effects		
			0	No evidence of developmental toxicity potential		
Toxic Chemical Release Inventory Risk Screening Guide (USEPA 1989, prepared by the Office of Toxic Substances, Volume 1, July)	Acute RQ	Ranking	Inhalation or Oral Rfd	Cancer or Chronic RQ	TPQ	Ranking
	<=100 lbs	Group 1	<0.01 mg/kg-day	Q1*	<=100 lbs =100 lbs	Group 1
	1,000	Group 2	0.01-0.1	All	1,000 500	Group 2
	5,000	Group 3	>=1.0		5,000 >=1,000	Group 3

Ranking Systems	Human Acute Toxicity	Human Chronic Toxicity	
Louisiana's Environmental Action Plan "Leap to 2000" (Public Advisory and Steering Committee Risk Ranking Retreat Briefing Material March 26, 1991)		Dose/Rfd	Score
		1-2	1
		2-10	2
		10-100	3
		> 100	4

Table 2: Environmental Toxicity Ranges

Ranking Systems	Aquatic Toxicity			Ecotoxicity			Mammalian Toxicity																										
Ranking the Relative Hazards of Industrial Discharges to POTWs and Surface Waters (USEPA 1989, prepared for OPA, February)	RQ  Used  Directly																																
Hazard Ranking System; Final Rule (55 Federal Register No. 241, pp. 51532-667, 12/14/90)				Surface Water:  <table><tr><td>Acute</td><td>Chronic</td><td></td></tr><tr><td>AWQC or</td><td>AWQC or</td><td>Assigned</td></tr><tr><td>AALAC</td><td>AALAC</td><td>Value</td></tr><tr><td>&lt; 1 µg/l</td><td>&lt; 100 µg/l</td><td>10,000</td></tr><tr><td>1-10</td><td>100-1,000</td><td>1,000</td></tr><tr><td>10-100</td><td>1,000-10,000</td><td>100</td></tr><tr><td>100-1,000</td><td>10,000-100,000</td><td>10</td></tr><tr><td>&gt; 1,000</td><td>&gt; 100,000</td><td>1</td></tr></table>			Acute	Chronic		AWQC or	AWQC or	Assigned	AALAC	AALAC	Value	< 1 µg/l	< 100 µg/l	10,000	1-10	100-1,000	1,000	10-100	1,000-10,000	100	100-1,000	10,000-100,000	10	> 1,000	> 100,000	1			
Acute	Chronic																																
AWQC or	AWQC or	Assigned																															
AALAC	AALAC	Value																															
< 1 µg/l	< 100 µg/l	10,000																															
1-10	100-1,000	1,000																															
10-100	1,000-10,000	100																															
100-1,000	10,000-100,000	10																															
> 1,000	> 100,000	1																															
TSCA Chemical Scoring System for Hazard and Exposure Evaluation	Life cycle Acute or Chronic <table><tr><td>LC50 or EC50</td><td>NOEL</td><td>Score</td></tr><tr><td>&lt; 1</td><td>&lt; 0.1</td><td>8-9</td></tr><tr><td>1-10</td><td>0.1-1</td><td>6-7</td></tr><tr><td>10-100</td><td>1-10</td><td>4-5</td></tr><tr><td>100-1,000</td><td>10-100</td><td>1-3</td></tr><tr><td>&gt; 1,000</td><td>&gt; 100</td><td>0</td></tr></table>			LC50 or EC50	NOEL	Score	< 1	< 0.1	8-9	1-10	0.1-1	6-7	10-100	1-10	4-5	100-1,000	10-100	1-3	> 1,000	> 100	0												
LC50 or EC50	NOEL	Score																															
< 1	< 0.1	8-9																															
1-10	0.1-1	6-7																															
10-100	1-10	4-5																															
100-1,000	10-100	1-3																															
> 1,000	> 100	0																															

Ranking Systems	Aquatic Toxicity			Ecotoxicity	Mammalian Toxicity	
Toxic Chemical Release Inventory Risk Screening Guide (USEPA 1989, prepared by the Office of Toxic Substances, Volume 1, July)	Aquatic					
	WQS	RQ	Ranking		TPQ	Ranking
	<= 100 lbs	<= 100 lbs	Group 1		<= 100 lbs	Group 1
	500	1,000	Group 2		500	Group 2
	>=1000 lbs	5,000	Group 3		> = 1,000	Group 3

Table 3: Exposure Parameter Ranges

Ranking Systems	Exposure Potential				Exposure Level	Population Level
Hazard Ranking	Surface Water:					
	Half Life	Half Life		Assigned		
	(Lakes)	(Other)	Log Kow	Value		
	< 0.02 days	< 0.2 days	< 3.5	0.0007		
	0.02-2	0.2-0.5	3.5-4	0.07		
	2-20	0.5-1.5	4-4.5	0.4		
	> 20	> 1.5	> 4.5	1		
	Surface Water:					
	Use priority: availability of BCF,					
	LogKow, water solubility					
	Assigned					
	Value	BCF	Log Kow	Water Solubility		
	50,000	> 10,000	5.5-6.0	< 25 mg/l		
	5,000	1,000-10,000	4.5-5.5	25-500		
	500	100-1,000	3.2-4.5	500-1,500		
	50	10-100	2.0-3.2	-		
	5	1-10	0.8-2.0	-		
	0.5	< 1	< 0.8	> 1,500		

Ranking Systems	Exposure Potential				Exposure Level	Population Level	
Hazard Ranking System: Final Rule (concluded)	Air:						
	Assigned						
	Vapor Pressure	Henry's Constant	Value				
	> 10 Torr	> 0.001 atm-m3/mol	3				
	10-0.001	10E-5 to 0.001	2				
	0.001-0.00001	10E-7 to 10E-5	1				
	< 0.00001	< 10E-7	0				
	Ground Water:						
	Water	Distribution Coefficient (Kd) (ml/g)					
	Solubility	Karst	< 10	10-1,000			> 1,000
	Liquid	1	1	0.01			0.0001
	> 100 mg/l	1	1	0.01			0.0001
	1-100	0.2	0.2	0.002			2.0e-05
0.01-1	0.002	0.002	2.0e-05	2.0e-07			
< 0.01	2.0e-05	2.0e-05	2.0e-07	2.0e-09			

Ranking Systems	Exposure Potential	Exposure Level	Population Level																								
USEPA Unfinished Business Report: A Comparative Assessment of Environmental Problems (USEPA, 1987, prepared by OPA, OAR, OAQPS, OW, and OSW, February)			<div>Non-Cancer Effects:</div> <table><tr><td>People Exposed</td><td>Score</td></tr><tr><td>&lt;1,000</td><td>1</td></tr><tr><td>1,000-10E5</td><td>2</td></tr><tr><td>10E5-10E7</td><td>3</td></tr><tr><td>&gt; 10E7</td><td>4</td></tr></table>	People Exposed	Score	<1,000	1	1,000-10E5	2	10E5-10E7	3	> 10E7	4														
People Exposed	Score																										
<1,000	1																										
1,000-10E5	2																										
10E5-10E7	3																										
> 10E7	4																										
TSCA's TRI Chemical Risk Assessment Pre-Screening Methodology TSCA's TRI Chemical Risk Assessment Pre-Screening Methodology (concluded)	<div>none = no expected release</div>	<table><tr><td>Criteria</td><td>Score</td></tr><tr><td>&gt; 700 mg/yr</td><td>3</td></tr><tr><td>70 to 700</td><td>2</td></tr><tr><td>&lt; 70</td><td>1</td></tr></table>	Criteria	Score	> 700 mg/yr	3	70 to 700	2	< 70	1	<div>Surface Water:</div> <table><tr><td>Criteria</td><td>Score</td></tr><tr><td>&gt; 10E6 people</td><td>3</td></tr><tr><td>10E5-10E6</td><td>2</td></tr><tr><td>&lt; 10E5</td><td>1</td></tr></table> <div>Ambient Air:</div> <table><tr><td>Criteria</td><td>Score</td></tr><tr><td>&gt; 10E5 people</td><td>3</td></tr><tr><td>10E4-10E5</td><td>2</td></tr><tr><td>&lt; 10E4</td><td>1</td></tr></table>	Criteria	Score	> 10E6 people	3	10E5-10E6	2	< 10E5	1	Criteria	Score	> 10E5 people	3	10E4-10E5	2	< 10E4	1
Criteria	Score																										
> 700 mg/yr	3																										
70 to 700	2																										
< 70	1																										
Criteria	Score																										
> 10E6 people	3																										
10E5-10E6	2																										
< 10E5	1																										
Criteria	Score																										
> 10E5 people	3																										
10E4-10E5	2																										
< 10E4	1																										

Ranking Systems	Exposure Potential	Exposure Level	Population Level
TSCA's TRI Chemical Risk Assessment Pre-Screening Methodology TSCA's TRI Chemical Risk Assessment Pre-Screening Methodology (concluded)			Ground Water:  CriteriaScore  > 25,000 people3  5,000-25,0002  < 5,0001
California Air Resource Board Toxic Chemical List & NIOSH/OSHA Pocket Guide (Air Resources Board of the State of California)	Air:  Dangerous:  IDLH < 2000 ppm  and  vapor pres. > 20 mmHg		
A Ranking System for Clean Water Act Section 307(a) List of Priority Pollutants (USEPA 1985, July)	Hydrolysis  Half LifeRateScore  > 12 mo-8  6-12 mo-5  3-6 mo> 3 mo2  48 hr - 3 mo48 hr - 3 mo0  24-48 hr< 48 hr-5  < 24 hr-8		

Ranking Systems	Exposure Potential			Exposure Level	Population Level
A Ranking System for Clean Water Act Section 307(a) List of Priority Pollutants (USEPA 1985, July)	Henry's				
	Constant	KD value	Score		
	< 10E-3	< 0.01	2		
	0.001-0.01	10E2-10E4	0		
	> 0.01	> 10E4	-5		
	BAF				
		Log P	Score		
	< 4,000	< 6	8		
	700-4,000	4.5-6	5		
	300-700	4-4.5	2		
> 300	>4	0			
TSCA Chemical Scoring System for Hazard and Exposure Identification (O'Bryan, T.R. and Ross, R.H. 1988, Journal of Toxicology and Environmental Health, Vol (1):119-134)	Half-life				
	Score				
	> 1 yr		5		
	8-52 wk		4		
	2-8 wk		3		
	1-14 days		2		
	< 1 day		1		
	BCF				
		Log P	Score		
	> 1,000	> 4.35	9		
	200-1,000	3.5-4.35	7		
	100-200	3.18-3.5	5		
	10-100	2.0-3.18	3		
	< 10	< 2.0	0		

Ranking Systems	Exposure Potential	Exposure Level	Population Level	
Louisiana's Environmental Action Plan "Leap to 2000" (Public Advisory and Steering Committee Risk Ranking Retreat Briefing Material, March 26, 1991)			Population Exposed	Score
			1-400	1
			400-4,000	2
			4,000-40,000	3
			40,000-400,000	4
			> 400,000	5
Screening Procedure for Chemicals of Importance to the Office of Water (USEPA 1987, prepared by OPA, OAR, OAQPS, OW, and OSW, February)	For human and aquatic populations:  BCF                      Score  > 1,000                High  < 1,000                Low			

Table 4: Severity of Measured Effects

Ranking Systems	Severity of Effect		
Examination of the Severity of Toxic Effects and Recommendation of a Systematic Approach to Rank Adverse Effects (USEPA 1986, prepared for ECAO, March)	Organ	Histopathological Severity	Toxicity Endpoint
	Loss of which is fatal and are irreplaceable (I) = 1.5	No change = 1.0	Body wt. change, food and/or water cons. change, impairment of organs (IV) = 1.0
	Loss of which may be fatal yet are replaceable or organs which are necessary for proper function of immunity (II) = 1.0	Effects evident only at EM level = 2.0	Small hematological changes, impairment of organs (III), weight change in organs (II, III, IV) = 2.0
	Loss of which is not fatal but may result in functional or emotional handicap (III) = 0.5	Swelling, degeneration, fatty change, pigment = 3.0	mild impairment of organs (II), severe impairment of organs (III), minor organ weight change (I) = 3.0
	Not found in humans and toxic lesions found may not transfer to humans (IV) = 0.25	Atrophy, hypertrophy, cytomegaly, hemorrhage = 4.0	mild impairment of organs (I), major impairment of organs (II), major organ weight change (I) = 4.0
		Necrosis, mineralization, emphysema, infarction = 5.0	Functional impairment of organs (I), = 5.0
		Fibrosis/regeneration, atypia hyperplasia/proliferation = 6.0	Major degree of funct'l impairment in organs (I) = 6.0
		Teratogenesis with maternal toxicity, fetotoxicity w/o maternal toxicity = 7.0	Nervous System, respiratory, or cardiovascular depression, mortality, developmental toxicity w/o maternal toxicity = 7.0
		Teratogenesis w/o maternal toxicity = 8.0	

Ranking Systems	Severity of Effect
<p>USEPA Unfinished Business Report: A Comparative Assessment of Environmental Problems (USEPA 1987, prepared by OPA, OAR, OAQPS, OW, and OSW, February)</p>	<p>Ranking of Organs</p> <p>Category I Includes organs, impairment or loss of which is fatal and cannot be compensated for at all, or only heroic measures (i.e. expensive mechanical devices, transplantation). Also includes gonads, loss of which prevents reproductions. Lung, heart, brain/spinal cord, kidney, liver, bone marrow, gonads</p> <p>Category II Includes organs whose loss or impairment may be fatal, but which can be compensated for by replacement therapy. Also includes organs, impairment or loss of which indicates as adverse effect on immune function or hematopoietic function which may be life threatening. Adrenal, thyroid, parathyroid, pituitary, pancreatic islets, pancreas, esophagus, stomach, small intestine, large intestine, lymph node, spleen, thymus, trachea, pharynx, urinary bladder, skin</p> <p>Category III Impairment or loss of any of these organs is not life threatening but may result in severe functional or emotional handicaps. Accessory reproductive organs (oviduct, epididymis, uterus, prostate, coagulating gland, seminal vesical, ductus deferens, penis, vagina), eye, bone, nose, nerve, muscle, urinary bladder, blood vessel, ear, gall bladder, harderian and lacrimal gland, larynx, mammary gland, salivary gland, tongue, tooth, ureter, urethra</p> <p>Category IV These organs are not found in humans and toxic lesions (noncarcinogenic) in these organs are not readily extrapolable to humans. Clitoral/preputial gland, zymbal's gland, anal glands</p>

#### **D. FACTORING DATA QUALITY/UNCERTAINTY INTO THE INDEX**

There are differences among chemicals in the supporting health effects and exposure data. Health data for one type of effect (e.g., cancer) may be based on animal studies, while evidence of other types of effects may be derived from epidemiology (e.g. neurological effects of lead). Even specific numerical estimates of a single type of effect, cancer potency, have varying levels of evidence to support the estimate. For some chemicals without any specific toxicity data, other information, such as structure-activity relationships, could be used to estimate the relative rankings. There will also be differences in levels of uncertainty associated with exposure scenarios. For example, it may be possible to model air and water emissions from certain facilities, but have less information on releases from TSDFs and POTWs.

One system reviewed that attempted to measure and incorporate any element of data uncertainty was the method for determining carcinogenicity RQ. This system employs an ordinal scoring for carcinogenic weight-of-evidence. This score is combined with a score based on  $q_1^*$  using a matrix in which each cell is assigned a high, medium or low rank. This same approach could be used to weight ranks in the noncancer toxicity categories, as well as in exposure categories. Alternatively, numerical uncertainty scores could be used to adjust chemical scores within a category.

#### **E. USING SEVERITY INDICES TO WEIGHT CHEMICAL SCORES WITHIN A CATEGORY**

Several systems develop human health effects scores that are comparable across different kinds of non-cancer risks. These systems employ effect severity indices to weight different effects by the relative risks they pose. For example, a report done for EPA/ECAO develops two scales that ordinarily rank noncarcinogenic toxic effects, one by lesion severity, another by type of effect. Both scales rank the effects relative to each other, but do not measure the magnitude of the overall risk. No attempt was made to rank these effects relative to cancer; nor did the report focus on reproductive or mutagenic effects. These scales would therefore be useful for ranking only noncarcinogenic human health risks.

#### **F. RANKING INDIVIDUAL CHEMICALS FOR TOXICITY OR FORMING SUBINDICES**

Once chemicals are scored relative to one another within each category, each chemical can be characterized by its profile of scores. At this point, a chemical's scores can be combined across categories to form a rank for that chemical in each area of interest (e.g., cancer risk, noncancer risk, environmental risk). These ranks would be used to calculate the Indicator. One advantage to this method is that such ranks indicate the relative importance of a chemical with a single number. Many systems, however, do not aggregate scores across categories (see the Region 7 and the OTS/ORNL scoring systems) because this requires making the difficult judgement about the relative importance of different kinds of risk.

Alternatively, scores can be aggregated within a category across chemicals to form a category subindicator. For example, mammalian acute toxicity scores of all chemicals might be added together

(possibly weighted by exposure scores) to calculate the 'mammalian acute toxicity subindex.' This could be done for each category, creating an aggregate profile of all of the TRI chemicals. Movements within these subindices would provide measures of environmental improvement.

#### **G. METHODS OF ESTABLISHING THE RELATIVE IMPORTANCE OF RISKS AMONG CATEGORIES**

If a single rank is to be calculated for each chemical from the various categorical scores, one of several calculation methods could be used. The simplest ways to combine numerical scores is to multiply or add them together. The flaw in this approach is that ordinal scores have no specific numerical meaning except within the categories, and even then they do not reflect the magnitude of the differences, but only the order of the ranks (see above.)

Another approach is to scale the scores then multiply or add them together so that the scores have a common denominator. For example, we could divide the exposure value at a facility by the maximum exposure value observed over all facilities. We can then add the scores in different categories because they have a similar scale.

A third approach is to create a matrix of categories and then rank each cell of the matrix separately. The cells may (but do not have to) reflect a mathematical function of the individual ranks of row and column that make up the cell. In this approach, individual chemicals would not be ranked; only the categories into which they fell would have ranks. This method is particularly appropriate for combining several qualitative (i.e. high, medium, low) scores. For example:

Aquatic Risk Rank		Persistence			
		0	1	2	3
Acute Aquatic Toxicity	Low	0	0	0	0
	Medium	3	6	9	12
	High	6	9	12	15
	Very High	9	12	15	18

A fourth option is simply to select the worst score that a chemical has in any category and use that value as the chemical's rank. This would require that all of the scores be of the same type, i.e. qualitative or numerical. It also implies that scales of the scores can be equated. The methods for determining scores in each of the categories would have to meet these criteria.

Ranks in one category could also be conditional on a rank in a different category. For example, noncarcinogenic chronic toxicity might only be meaningful if exposure is above threshold RfD. Criteria for ranking a chemical might require that the noncarcinogenic toxicity score and exposure score meet separate criteria at the same time.

Special decision rules may be applied in conjunction with the overall scoring system. This may be useful in cases in which a particular score category is of overwhelming importance given certain conditions. For example, an extreme carcinogenicity score, regardless of other scores, might automatically classify a chemical as "high". A *de minimis* emissions score might eliminate the chemical from further consideration regardless of toxicity scores. Chemicals with very low toxicity in all categories might also be eliminated.

#### **H. WEIGHTING SCORES: AN ALTERNATIVE TO METHODS PRESENTED IN I.G.**

One option discussed in Section I.e. was to combine scores across categories to derive a single score for the chemical. A scoring algorithm to combine a chemical's scores across categories into a single rank requires the assignment of weights to each of the scoring elements. This is probably the most controversial and difficult step in the process because of the difficulty in evaluating the relative importance of different kinds of risk. In fact, some of systems we reviewed avoided this step altogether. However, in order to develop a single index that encompasses different kinds of risk (e.g. a human health index which incorporates both carcinogenic and noncarcinogenic risks), a weighting system which implies relative importance of effects will have to be used.

The primary issue in comparing two risks of different nature centers on attributing a common unit of value to the risks so that their relative magnitude can be compared. Of the EPA and non-EPA ranking systems reviewed under this assignment, only the Office of Toxic Substances Production-Based Targeting Methodology explicitly assigns relative values to different kinds of risks. Risks from oncogenicity, reproductive and neurotoxicity, chronic toxicity, and ecotoxicity were assigned relative weights of 3, 1, 2 and 2, respectively. Outside of the Agency, Louisiana's Environmental Action Plan gave equal weight to human cancer and non-cancer risks.

Other ranking systems implicitly weight different toxicity risks. For example, RQs indirectly address disparate risk comparisons by restricting the possible scores depending on the particular RQ being developed: cancer RQs can only range from 1-100, while aquatic toxicity RQs can range from 1-5000. The Hazard Ranking System employs a toxicity scale from 0 to 10,000 that enters into the calculation of site ranking without adjustment for the kind of toxic risk measured. The scale is based on various measures depending on the kind of toxicity being incorporated:

Human Chronic Toxicity	Human Carcinogenicity			Acute Human Toxicity				Assigned Value
Reference dose (RfD) (mg/kg-day)	Weight-of-Evidence and Slope Factor (SF) (mg/kg-day)			Oral LD <sub>50</sub> (mg/kg)	Dermal LD <sub>50</sub> (mg/kg)	Dust or mist LC <sub>50</sub> (mg/l)	Gas or Vapor LC <sub>50</sub> (ppm)	
	A	B	C					
< 0.0005	0.5 <	5 <	50 <	NA	NA	NA	NA	10,000
0.0005 to 0.005	0.5 to 0.05	<b>5 to 0.5</b>	50 to 5	< 5	< 2	< 0.2	< 20	1,000
<b>0.005 to 0.05</b>	< 0.05	0.5 to 0.05	5 to 0.5	5 to 50	2 to 20	0.2 to 2	20 to 200	100
0.05 to 0.5	NA	< 0.05	< 0.5	50 to 500	20 to 200	2 to 20	200 to 2,000	10
0.5 <	NA	NA	NA	500 <	200 <	20 <	2,000 <	1

This system implies that risk from a class B carcinogen with a slope factor between 5 and 0.5 is ten times greater than the risk posed by a chronic toxic effect with an RfD between 0.005 and 0.05. The 307(a) Priority Pollutant Chemical Ranking System employs a similar method to develop toxicity scores.

There are also several approaches described in the economics literature that could be used to develop the relative severity ranking. First, economists use various techniques to determine the willingness to pay to avoid various health effects. Other studies examine direct risk/risk tradeoffs. One methodology involves asking respondents to choose between a number of hypothetical scenarios, two at a time. A point of indifference can be established between two scenarios through multiple iterations of questioning. This value determines a relative weight for the health effect being measured. Another method, the health status index, measures health effects in terms of changes in quality of life. While the scope of this project does not allow for original research, we could examine the available economics literature for results that would be applied in this context.

## II. Options for Ranking of Chemicals

Section I has described the elements of a scoring system. The components described in that section can be combined in numerous ways to produce an index. The following is a discussion of three possible options. **The options presented below should in no way be considered the universe of possible options.** Rather, they should be considered as points of departure for discussion of an appropriate algorithm for constructing the TRI index. The elements of each of the options were drawn from (or are modifications of) scoring systems discussed in the review memorandum entitled "Previous Work on Scoring Systems and Chemical Indices." However, none of the options presented below follows one system in its entirety; the specific combinations of components are original to this exercise. Option 1 ranks chemicals ordinally, based on selected measures of the toxicity and exposure potential of a chemical. These ranks are combined with population and emissions data to determine the final TRI indicator. Option 2 takes the same general approach but instead of ordinal ranks uses actual toxicity data values to develop unique rankings for each chemical. Option 2 also uses modelling to evaluate exposure potential. Option 3 describes an approach where categories of chemicals are defined based on relevant toxicity and exposure potential combinations. The categories (rather than the chemicals themselves) are assigned relative ranks. Chemicals are then assigned to the categories. Site-specific population and emissions data are then combined with the categorical ranks to calculate the indicator.

Step-by-step descriptions of each of these options are presented below. For each step, we identify previous EPA or other scoring systems that have used similar approaches. Summaries of other EPA and non-EPA scoring systems are presented in the memorandum entitled "Previous Scoring and Ranking Systems" (hereafter referred to as the scoring system review memo). To illustrate the use of these options, we have created a sample data set of six hypothetical chemicals and three hypothetical facilities. The chemical-specific and site-specific data for these six chemicals are shown in Tables 5 and 6. For each of the options proposed, we provide an example of how the indicator would be constructed based on the sample data set.<sup>2</sup> The sample data set is kept simple intentionally, since our current focus is the conceptual structure of the indicator rather than the vagaries of our data set. Of course, the actual data set will be far more complicated, uncertain and incomplete than the sample data presented here. Once the Work Group has had the opportunity to review and discuss the conceptual approaches, we can explore the details of implementing potential options using an actual subset of the TRI data set.

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<sup>2</sup> While the examples provided show how a human-health based indicator would be developed, the same principles can be applied to the development of an ecological indicator.

Table 5: Chemical Specific Data

Chemical	Toxicity Data				Physicochemical Data						
	Cancer		Chronic Toxicity Other Than Cancer		Volatility		Partitioning			Persistence	
	WOE	q1* (kg-day/mg)	RfD (mg/kg-day)	Chronic Effect of Concern	Vapor Pressure (torr)	Henry's Law Constant (atm-m3/mol)	Koc (cm3/g)	BCF	Solubility (mg/l)	Photolysis (1/hr)	Hydrolysis (1/hr)
A	B2	10	0.1	liver hypertrophy	3.00e+03	2.00e-07	4.00e+01	10	4.00e+05	5.00e-03	6.80e-05
B	B2	0.001	0.2	nerve damage	1.00e+02	2.00e-02	2.00e+02	50	8.00e+02	3.00e-08	4.00e-08
C	B2	1	0.02	spontaneous abortion	4.00e-03	1.00e-05	1.10e+03	200	5.00e+00	4.00e-03	4.00e-02
D	A	0.03	0.05	liver toxicity	4.00e-04	1.00e-03	3.00e+03	1000	2.00e-01	1.00e-05	7.00e-03
E (metal)	C	5	0.005	slowed neural response	0	0	na	0	5.00e-01	0	0
F (metal)	B2	45 (I)	0.001	decreased spermatogenesis	0	0	na	0	5.00e+01	0	0

Table 6: Site-Specific Exposure Data

Facility and Chemicals	Emissions		Population Exposed		Characteristics of Facility	
	Air (lbs/yr)	Water (lbs/yr)	Air (no. people)	Water (no. people)	Air	Water
Facility 1						
A	1000	6000	3000	500	High Dispersion	Low
B	2000	4000	3000	500		Stream
C	2000	1000	3000	500		Flow
E	4000	3000	3000	500		
Facility 2						
C	3000	1000	1000	6000	Low Dispersion	Medium
D	4000	5000	1000	6000		Stream
F	10000	2000	1000	6000		Flow
Facility 3						
A	2000	4000	2000	2000	Medium Dispersion	High
C	4000	2000	2000	2000		Stream
D	6000	10000	2000	2000		Flow
E	1000	6000	2000	2000		

## Option 1.

### **Step 1. Using an ordinal scale, rank chemicals within each toxicity evaluation criterion.**

Ordinal ranking is a common approach in a number of ranking systems. Often, ranks are assigned on an ordinal scale (from 0-10, for example) rather than assigning unique values to each chemical. The ranking of the chemicals is based on quantitative dose-response information if possible. Several systems we reviewed used ordinal scales for ranking toxicity, including the TRI Risk Screening Guide, OTS pollution prevention screening, the OTS/ORNL chemical ranking scheme, and the Louisiana Environmental Action Plan.

**Step 2a. Within each of these toxicity categories, assign severity rank (e.g., cellular change versus organ damage) for noncarcinogens.** Chemicals that have similar reference doses may pose dissimilar health risks. Severity ranking attempts to weight chemicals based on the relative gravity of the noncancer health effects risks posed. Severity ranking has been used in several previous ranking/scoring efforts, such as the OTS pollution prevention screening, the Integrated Environmental Management Program, and the Louisiana Environmental Action Plan. A scheme for severity ranking was presented in the ECAO report entitled "Examination of the Severity of Toxic Effects and Recommendations of a Systematic Approach to Rank Adverse Effects," which is presented in detail in the scoring systems review memo.

**Step 2b. Assign ranks based on weight-of-evidence (e.g., substantial evidence versus suggestive evidence) ranks for carcinogens.** This step is an attempt to recognize the uncertainty in the classification of a chemical as a human carcinogen. This step uses the CAG weight-of-evidence (WOE) classification scheme (where A = known human carcinogen; B = probable human carcinogen; and C = possible human carcinogen) to weight carcinogens. Ranking based on weight-of-evidence classification has been used in the OTS pollution prevention screening and in the Integrated Environmental Management Program, and has played a role in other schemes that use "best professional judgment" to assign ranks to chemicals (such as the Unfinished Business report).

**Step 3. Determine relative weights for each toxicity category relative to other categories (e.g., hepatic effects versus cancer).** This is likely to be among the most controversial steps in the process. Many scoring systems have avoided combining dissimilar risks and have instead developed separate scores for different types of risks. For example, the Region VII TRI strategy is to derive separate indices for chemicals based on acute effects, chronic noncancer, cancer and aquatic toxicity. However, a few weighting schemes (notably, two regulatory efforts) have compared different types of toxicity. The Hazard Ranking System (used to place sites on the NPL) implicitly assigns relative weights to cancer and non-cancer effects by using the same scale to score chemicals on these attributes (see the scoring systems review memo for further detail). Also, OAQPS has proposed a scheme for establishing off-setting emissions credits in the program governing early emissions reductions of hazardous air pollutants. The scheme explicitly allows emissions trading among carcinogens and other chemicals, where emissions from carcinogens are (numerically) weighted more heavily than noncarcinogens.

**Step 4. The categorical toxicity rank for each chemical is the product of the raw toxicity rank, the severity/WOE rank and the categorical rank. The overall toxicity rank for a chemical is the average of its ranks in the four toxicity categories.** Another possible approach would be to take the root mean square of the four toxicity category ranks (an approach used in the Hazard Ranking System).

**Step 5. For the exposure evaluation criteria, use photolysis rate, solubility, and bioconcentration factor to rank chemicals for the inhalation, drinking water, and fish ingestion exposure pathways, respectively.** A number of systems use relevant physicochemical values to evaluate exposure potential in various media. The Risk Screening Guide used selected physicochemical parameters to qualitatively evaluate mobility of chemicals in each media. The Hazard Ranking System also uses selected parameters to score exposure potential, although a greater number of parameters are included in the HRS exposure evaluation because some site-specific data are generally available for HRS evaluations.

**Step 6. Multiply the media-specific exposure rank and toxicity rank by population exposed and emissions for that pathway for each facility.** This step combines the toxicity considerations with the factors that determine exposure potential (i.e., the chemical's exposure rank and emissions, and population size). Size of exposed population is used as a ranking criterion in many of scoring systems we reviewed, including: the PPD TRI pollution prevention targeting; OPA ranking of discharges to POTWs and surface waters; OTS TSCA prescreening of TRI chemicals; the Hazard Ranking System; the Integrated Environmental Management Program; the Louisiana Environmental Action Plan; and the California Air Toxics Hotspots Program.

The use of population size as a prominent weighting factor may be unacceptable to those who feel that such an emphasis undervalues risks to rural populations. Furthermore, various regulatory efforts in the Agency focus risks to the Most Exposed Individual (MEI); a TRI indicator method which does not consider MEI risks would conflict with this philosophy. There are also difficulties associated with characterizing the size of exposed populations for certain exposure pathways (such as solid waste disposal). These difficulties will result in unequal levels of uncertainty in the exposure potential evaluation across exposure pathways.

On the other hand, overall population risk has been used elsewhere (notably, in the Unfinished Business report) to characterize general environmental progress; avoidance of population risk, not MEI risk, is also used in cost-benefit analyses to describe potential benefits of implementing environmental regulations.

**Step 7. The final index is the sum of the weighted volumes for all TRI chemicals for all pathways across all facilities.**

A step-by-step example demonstrating Option 1 for the sample data set is found in **Figure 1**.

**Advantages** - This option allows fine-scale tracking of subtle differences among chemicals. Importantly, by calculating media-chemical-facility subindices, we can easily identify underlying reasons for changes in the overall index by tracking individual media, industries, or chemicals. However, the final calculation yields a single index rather than a series of subindices across categories that may be hard for the public to interpret.

**Disadvantages** - Determining appropriate and sensible weighting factors for the different elements is difficult. Retaining a proportional scoring system based largely on ordinal ranks and performing mathematical functions on them may give the false impression that the absolute magnitude of the ranks have numerical meaning.

### Figure 1. Example Calculation for Option 1 Ranking System

Step 1. Using an ordinal scale, rank chemicals within each selected toxicity evaluation criteria.

For this and subsequent steps, ranks are ordered low to high.

Chemical	Cancer	Chronic Toxicity Other Than Cancer		
		Liver	Neurologic	Reproductive
A	5	1		
B	1		1	
C	3			1
D	2	2		
E (metal)	4		2	
F (metal)	6			2

Step 2. Within each of these categories, assign severity and weight of evidence rank to each chemical.

2.a. For this step, we use weights from 1 to 3 to rank the relative severity of chronic effects.

Chemical	Chronic Toxicity Other Than Cancer		
	Liver	Neurologic	Reproductive
A	1		
B		3	
C			2
D	3		
E (metal)		1	
F (metal)			1

2.b. We use weights from 1 to 3 for assigning carcinogens by their weight of evidence classification.

Chemical	Cancer (WOE)
A	2
B	2
C	2
D	3
E (metal)	1
F (metal)	2

Step 3. Determine weights for each toxicity category.

For the purposes of this example, the relative weights are:

Cancer	10
Reproductive Effects	7
Neurological Effects	5
Other Chronic Effects	2

Step 4. Derive categorical toxicity rank by multiplying toxicity rank, effect-specific severity rank, weight of evidence rank and cross-category severity rank. To get overall rank, average the chemical's rank in each category.

Chemical	Cancer (a)	Chronic Toxicity Other Than Cancer (b)			OVERALL AVERAGE (a+b)/2
		Liver	Neurologic	Reproductive	
A	$5 \times 2 \times 10 = 100$	$1 \times 1 \times 2 = 2$			51
B	$1 \times 2 \times 10 = 20$		$1 \times 3 \times 5 = 15$		17.5
C	$3 \times 2 \times 10 = 60$			$1 \times 2 \times 7 = 14$	37
D	$2 \times 3 \times 10 = 60$	$2 \times 3 \times 2 = 12$			36
E (metal)	$4 \times 1 \times 10 = 40$		$2 \times 1 \times 5 = 10$		25
F (metal)	$6 \times 2 \times 10 = 120$			$2 \times 1 \times 7 = 14$	67

Step 5. Derive Rank for each exposure pathway based on salient physicochemical parameter.

Chemical	Air	Drinking Water	Fish Ingestion
	Based on Photosynthesis	Based on Solubility	Based on BCF
A	1	6	3
B	4	5	4
C	2	3	5
D	3	1	6
E (metal)	5	2	1
F (metal)	5	4	1

Step 6. Combine exposure and toxicity ranks with population and emissions data to obtain media-specific indices.

Facility	Chemical	Emissions (lbs/yr) (a)	Pop. Exposed (no. people) (b)	Toxicity Rank (c)	Exposure Rank (d)	AIR INDEX $e=abxcxd$
Facility 1	A	1000	3000	51	1	1.5E+08
Facility 3	A	2000	2000	51	1	2.0E+08
Facility 1	B	2000	3000	17.5	4	4.2E+08
Facility 1	C	2000	3000	37	2	4.4E+08
Facility 2	C	3000	1000	37	2	2.2E+08
Facility 3	C	4000	2000	37	2	5.9E+08
Facility 2	D	4000	1000	36	3	4.3E+08
Facility 3	D	6000	2000	36	3	1.3E+08
Facility 1	E	4000	3000	25	5	1.5E+09
Facility 3	E	1000	2000	25	5	2.5E+08
Facility 2	F	1000	1000	67	5	3.4E+09
TOTAL:						8.9E+09

FOR WATER:

We obtain an average rank for water exposures using the following formula:

Total exposure to water sources is expressed as : 2L drinking water + [0.14 kg fish x BCF (L/kg)]

Average rank for water = (Rank for drinking water x (2 L/total exp.)) + (Rank for fish x (0.14 x BCF)/total exp.)

Facility	Chemical	Emissions (lbs/yr) (a)	Pop. Exposed (no. people) (b)	Toxicity Rank (c)	Drinking Water Exposure Rank (d)	Fish Ingestion Exposure Rank (e)	BCF Value (f)	Average Water Rank (g)=(d)x2L/tot exp +(e)x0.14(f)/tot exp	WATER INDEX h=axbxcxg
Facility 1	A	6000	500	51	6	3	10	5	7.3E+08
Facility 3	A	4000	2000	51	6	3	10	5	1.9E+09
Facility 1	B	4000	500	17.5	5	4	50	4	1.5E+08
Facility 1	C	1000	500	37	3	5	200	5	9.0E+07
Facility 2	C	1000	6000	37	3	5	200	5	1.1E+09
Facility 3	C	2000	2000	37	3	5	200	5	7.2E+08
Facility 2	D	5000	6000	36	1	6	1000	6	6.4E+09
Facility 3	D	10000	2000	36	1	6	1000	6	4.3E+09
Facility 1	E	500	500	25	2	1	0	2	7.5E+07
Facility 3	E	2000	2000	25	2	1	0	2	6.0E+08
Facility 2	F	6000	6000	67	4	1	0	4	3.2E+09
TOTAL:									1.9E+10

Step 7. Sum media-specific indices for overall TRI index.

Facility	Chemical	AIR INDEX (a)	WATER INDEX (b)	TOTAL INDEX c=(a+b)
Facility 1	A	1.5E+08	7.3E+08	8.8E+08
Facility 3	A	2.0E+08	1.9E+09	2.1E+08
Facility 1	B	4.2E+08	1.5E+08	5.7E+08
Facility 1	C	4.4E+08	9.0E+07	5.3E+08
Facility 2	C	2.2E+08	1.1E+09	1.3E+09
Facility 3	C	5.9E+08	7.2E+08	1.3E+09
Facility 2	D	4.3E+08	6.4E+09	6.8E+09
Facility 3	D	1.3E+09	4.3E+09	5.6E+08
Facility 1	E	1.5E+09	7.5E+07	1.6E+09
Facility 3	E	2.5E+08	6.0E+08	8.5E+08
Facility 2	F	3.4E+09	3.2E+09	6.6E+09
TOTAL:		8.9E+09	1.9E+10	2.8E+10

## Option 2.

**Step 1. Rank chemicals using actual proportional measures for the categories of concern.** For carcinogens, use  $q_1^*$  values. The  $q_1^*$  expresses risk to an individual per milligram (mg) of chemical per kilogram of body weight per day (mg/kg-day). For noncarcinogens, use the inverse of the RfD. The RfD is the dose (expressed as mg of chemical per kg body weight per day) below which no adverse effects are expected to occur. Using proportional measures for toxicity ranking is a common approach in other ranking systems. For example, RQs were used by OPA in ranking discharges to POTWs and to surface water bodies; OTS TSCA prescreening of TRI chemicals used RQ as a cutoff for high concern chemicals. RfDs and  $Q^*$  are proposed as the basis for toxicity ranking in Region VII's TRI strategy. Outside the Agency, the California Air Toxic Hotspots program uses actual dose-response data (in conjunction with exposure modelling - discussed below) in their identification and ranking of air toxics problems in the state.

**Step 1a. Since toxicity values in different categories have dissimilar units (e.g., cancer potency estimate versus an RfD), normalize the values by expressing the chemical's toxicity value in a given category as a fraction of the maximum value possible in that category.** The resulting fraction is the chemical's rank in that category. Expressing the ranks in this manner will also allow us to combine the ranks with exposure potential ranks that have been normalized in a similar manner (see below). This normalizing approach was used in OAQPS' Source Category Ranking System, which ranks potential air toxics problems across industries.

Once the toxicity ranks within categories are determined, the next three steps are the same as those described in Option 1.

**Step 2a and 2b. Within each toxicity category, assign severity and weight-of-evidence (WOE) ranks to each chemical.**

**Step 3. Determine relative weights for each toxicity category relative to other categories.**

**Step 4. Determine the categorical toxicity rank for each chemical.** The categorical rank is the product of the raw toxicity rank, the severity rank, the WOE rank and the categorical rank. The overall toxicity rank is the average of its ranks in the four toxicity categories.

**Step 5. For the exposure evaluation, model the fate and transport of the chemicals.** To do so, use the emissions data, site-specific environmental characteristics (or default values where these are not available), and physicochemical properties to obtain ambient media concentrations at specified distances. These data can be weighted by the number of persons at each distance (that is, the number of persons exposed to each estimated concentration) to obtain population-weighted average exposures for each site where chemical is emitted.

As mentioned earlier, specific methods for applying exposure modelling to the TRI database are discussed in a separate memo and will not be expanded on here. However, it should be noted that

generic exposure modelling to rank exposure potential is used by a number of other scoring/ranking systems. For example, Appendix B of the Risk Screening Guide presents results of generic air modelling to assist readers in the evaluation of air releases. OTS' TSCA prescreening of TRI chemicals used generic air and water exposure modelling to place chemicals in categories of low, medium and high concern. Furthermore, generic air modelling was used by OAQPS to identify high risk chemicals as part of defining offsets credits for early emissions reductions of hazardous air pollutants. Other scoring methods using generic modelling approaches include the California Air Toxics Hotspots program and OAQPS' Source Category Ranking System.

**Step 6. For each chemical-facility combination, express the exposure estimate as a fraction of the maximum exposure observed to obtain an exposure index.** Normalizing the exposure values allows us to combine the exposure ranks with the toxicity rankings in later steps. Otherwise, we would be combining ranks with dissimilar scales. The exposure index is then combined with the toxicity rank to derive the medium-specific index. The final index is the sum of the media-specific indices.

(A modification to this approach would be to use the RfDs and  $q_1^*$ s in concert with the exposure models to estimate cancer cases and/or number of individuals above the RfD. The "cases" could then be scaled by the maximum number of "cases" observed at each facility to obtain a unique subindex for each chemical-facility combination by exposure pathway. The index for the chemical would be the sum of the subindices across all facilities. The overall index would be the sum of the chemical indices.)

An example demonstrating Option 2 for the sample data set is found in **Figure 2**.

**Advantages** - The use of location-dependent exposure indices allows the index to reflect changes in where chemicals are released, as well as changes in volume. Normalizing toxicity ranks allows the use of structure-activity relationships to fill in data gaps; if a particular toxicity value is not known, the chemical can still be assigned a rank relative to the highest value in the category.

**Disadvantages** - The lack of toxicity data for many of the TRI chemicals would hinder this approach. This approach presents some programming challenges for performing multiple chemical, multiple site analyses. This option has the same difficulties as Option 1 in assigning appropriate sensible weighting factors to different elements. Furthermore, the option relies on normalizing the ranks based on a "reference chemical" which has the maximum value in the ranking category. A danger in this approach is the possibility that the underlying data (toxicity or physicochemical information) may change over time. Since all other chemical ranks are keyed to the values for this chemical, a change in the reference chemical would change the entire index. Therefore, rather than selecting the chemical with the maximum value, we may want to select as the reference chemical a well-known, well-characterized chemical for which underlying data is unlikely to change. Using this approach, the reference chemical rank would still be 1, while chemicals with values greater than the reference chemical would be assigned ranks proportionally greater than 1.

## Figure 2. Example Calculation for Option 2 Ranking System

Step 1. Using inverse of RfD value and actual  $q^*$  values, rank chemicals within each selected toxicity evaluation criteria.

For this and subsequent steps, ranks are ordered low to high.

Chemical	Cancer ( $q^*$ )	Chronic Toxicity Other Than Cancer (1/RfD)		
		Liver	Neurologic	Reproductive
A	10	10		
B	0.001		5	
C	1			50
D	0.03	20		
E (metal)	5		200	
F (metal)	45			1000

Step 1a. Since the raw toxicity ranks are on different scales, express the rank in each category as a fraction of the maximum rank observed in that category. The maximum rank is 1.

Chemical	Cancer	Chronic Toxicity Other Than Cancer		
		Liver	Neurologic	Reproductive
A	2.2E-01	0.5		
B	2.2E-05		0.025	
C	2.2E-02			0.05
D	6.7E-04	1		
E (metal)	1.1E-01		1	
F (metal)	1.0E+00			1

Step 2. Within each of these categories, assign severity and weight of evidence rank to each chemical.

2.a. As in Option 1, we use weights from 1 to 3 to rank the relative severity of chronic effects.

Chemical	Chronic Toxicity Other Than Cancer		
	Liver	Neurologic	Reproductive
A	1	3	2
B			
C			
D	3	1	1
E (metal)			
F (metal)			

2.b. We use weights from 1 to 3 for assigning carcinogens by their weight of evidence classification.

Chemical	Cancer (WOE)
A	2
B	2
C	2
D	3
E (metal)	1
F (metal)	2

Step 3. Determine severity weights for each toxicity category.

This step is also the same as Option 1. For the purposes of this example, the relative weights are:

Cancer	10
Reproductive Effects	7
Neurological Effects	5
Other Chronic Effects	2

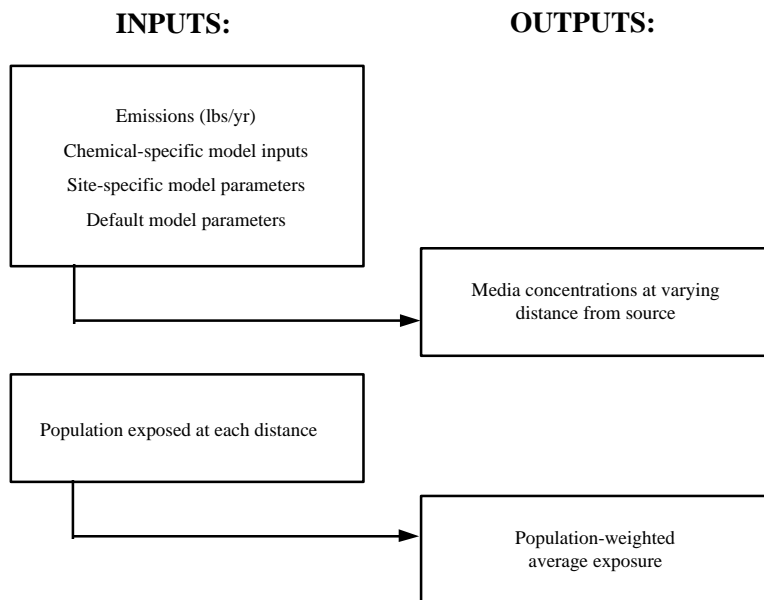
Step 4. Derive categorical toxicity rank by multiplying toxicity rank, severity rank and category rank. To get overall rank, average the chemical's rank in each category.

Chemical	Cancer (a)	Chronic Toxicity Other Than Cancer (b)			OVERALL AVERAGE (a+b)/2
		Liver	Neurologic	Reproductive	
A	$2e-1 \times 2 \times 10 = 4$	$0.5 \times 1 \times 2 = 1$			2.7
B	$2e-5 \times 2 \times 10 = 4e-4$		$0.025 \times 3 \times 5 = 4e-1$		0.2
C	$2e-2 \times 2 \times 10 = 4e-1$			$0.05 \times 2 \times 7 = 7e-1$	0.6
D	$7e-4 \times 3 \times 10 = 2e-2$	$1 \times 3 \times 2 = 6$			3.0
E (metal)	$1e-1 \times 1 \times 10 = 1$		$1 \times 1 \times 5 = 5$		3.1
F (metal)	$1 \times 2 \times 10 = 20$			$1 \times 1 \times 7 = 7$	13.5

Step 5. Derive rank for each exposure pathway using modelling approach.

For this step, we use computer programs to estimate population-weighted average in each medium, for each chemical at each facility.

The steps are as follows:



For the purposes of this example, we assume that these models yield the following results:

FOR AIR:

Facility	Chemical	Emissions (lbs/yr)	Pop. Exposed (no. people)	Population-Weighted Average Exposure (calculated with model)
Facility 1	A	1000	3000	5.0E-04
Facility 3	A	2000	2000	3.3E-03
Facility 1	B	2000	3000	9.0E-03
Facility 1	C	2000	3000	2.0E-03
Facility 2	C	3000	1000	3.3E-03
Facility 3	C	4000	2000	8.0E-03
Facility 2	D	4000	1000	3.3E-02
Facility 3	D	6000	2000	2.0E-02
Facility 1	E	4000	3000	2.0E-02
Facility 3	E	1000	2000	1.7E-02
Facility 2	F	10000	1000	1.7E-01

FOR WATER:

Facility	Chemical	Emissions (lbs/yr)	Pop. Exposed (no. people)	Population-Weighted Average Exposure (calculated with model)
Facility 1	A	6000	500	3.5E-02
Facility 3	A	4000	2000	9.4E-03
Facility 1	B	4000	500	1.2E-02
Facility 1	C	1000	500	2.9E-04
Facility 2	C	1000	6000	7.1E-04
Facility 3	C	2000	2000	4.7E-04
Facility 2	D	5000	6000	2.8E-02
Facility 3	D	10000	2000	4.7E-04
Facility 1	E	3000	500	1.8E-04
Facility 3	E	6000	2000	7.1E-03
Facility 2	F	2000	6000	7.1E-02

Step 5a. Take the exposures as a fraction of the maximum in order to get exposure indices for the chemicals.

FOR AIR:

Facility	Chemical	Exposure Index
Facility 1	A	3.0E-03
Facility 3	A	2.0E-02
Facility 1	B	5.4E-02
Facility 1	C	1.2E-02
Facility 2	C	2.0E-02
Facility 3	C	4.8E-02
Facility 2	D	2.0E-01
Facility 3	D	1.2E-01
Facility 1	E	1.2E-01
Facility 3	E	1.0E-01
Facility 2	F	1.0E+00

FOR WATER:

Facility	Chemical	Exposure Index
Facility 1	A	5.0E-01
Facility 3	A	1.3E-01
Facility 1	B	1.7E-01
Facility 1	C	4.2E-03
Facility 2	C	1.0E-02
Facility 3	C	6.7E-03
Facility 2	D	4.0E-01
Facility 3	D	6.7E-03
Facility 1	E	2.5E-03
Facility 3	E	1.0E-01
Facility 2	F	1.0E+00

Step 6. To derive media-specific indices, multiply toxicity ranks and exposure indices. To derive final index, add media-specific indices.

Facility	Chemical	Air Exposure Index (from Step 5a) (a)	Toxicity Rank (from Step 4) (b)	AIR INDEX  $c=(axb)$
Facility 1	A	3.0E-03	2.7	8.10E-03
Facility 3	A	2.0E-02	2.7	2.72E+00
Facility 1	B	5.4E-02	0.2	2.54E-01
Facility 1	C	1.2E-02	0.6	6.12E-01
Facility 2	C	2.0E-02	0.6	6.20E-01
Facility 3	C	4.8E-02	0.6	6.48E-01
Facility 2	D	2.0E-01	3	3.20E+00
Facility 3	D	1.2E-01	3	3.12E+00
Facility 1	E	1.2E-01	3.1	3.22E+00
Facility 3	E	1.0E-01	3.1	3.20E+00
Facility 2	F	1.0E+00	13.5	1.45E+01
TOTAL:				32.1

Facility	Chemical	Water Exposure Index (from Step 5a) (a)	Toxicity Rank (from Step 4) (b)	WATER INDEX  $c=(axb)$
Facility 1	A	5.0E-01	2.7	1.35E+00
Facility 3	A	1.3E-01	2.7	2.83E+00
Facility 1	B	1.7E-01	0.2	3.67E-01
Facility 1	C	4.2E-03	0.6	6.04E-01
Facility 2	C	1.0E-02	0.6	6.10E-01
Facility 3	C	6.7E-03	0.6	6.07E-01
Facility 2	D	4.0E-01	3	3.40E+00
Facility 3	D	6.7E-03	3	3.01E+00
Facility 1	E	2.5E-03	3.1	3.10E+00
Facility 3	E	1.0E-01	3.1	3.20E+00
Facility 2	F	1.0E+00	13.5	1.45E+01
TOTAL:				33.6

Facility	Chemical	AIR INDEX (a)	WATER INDEX (b)	OVERALL INDEX  c=(a+b)
Facility 1	A	8.10E-03	1.35E+00	1.4
Facility 3	A	2.72E+00	2.83E+00	5.6
Facility 1	B	2.54E-01	3.67E-01	0.6
Facility 1	C	6.12E-01	6.04E-01	1.2
Facility 2	C	6.20E-01	6.10E-01	1.2
Facility 3	C	6.48E-01	6.07E-01	1.3
Facility 2	D	3.20E+00	3.40E+00	6.6
Facility 3	D	3.12E+00	3.01E+00	6.1
Facility 1	E	3.22E+00	3.10E+00	6.3
Facility 3	E	3.20E+00	3.20E+00	6.4
Facility 2	F	1.45E+01	1.45E+01	29.0
TOTAL:		32.1	33.6	65.7

### Option 3.

**Step 1. From among the various toxicity categories, choose the category which yields the lowest dose.** This is the limiting dose. This decision rule was used in the ranking of chemicals for inclusion as priority pollutants under the Clean Water Act.

**Step 2. Establish criteria for placing chemicals in categories of low, medium and high toxicity based on the limiting dose, and classify chemicals based on these criteria.** A number of scoring systems have provided criteria that could be used to place chemicals in categories of low, medium and high concern. The human and environmental toxicity categories into which chemicals were divided and the criteria used to place chemicals in these categories for each scoring system were summarized in Tables 1 and 2 of this memo.

**Step 3. To assess exposure potential, use photolysis rate, solubility, and bioconcentration factor for the inhalation, drinking water, and fish ingestion exposure pathways, respectively to place chemicals in categories of low, medium and high for exposure potential. Classify chemicals based on these criteria.** As with the toxicity ranking, a number of scoring systems have provided criteria that could be used to place chemicals in categories of low, medium and high exposure potential. The exposure potential categories into which chemicals were divided and the criteria used to place chemicals in these categories for each scoring system were summarized in Table 3 of this memo.

**Step 4. Construct human hazard and exposure potential matrices for each medium of concern; assign chemicals to each cell according to their toxicity and medium-specific classifications.** An example of such a matrix is given in ORD's "Simplified Approach for Screening and Categorizing Toxic Chemicals." A toxicity/exposure matrix was also used in the University of Michigan's application of the Hazard Ranking System to the prioritization of organic compounds at hazardous waste sites.

**Step 5. Assign weights to the low, medium and high categories for exposure potential and toxicity.** In our example, the rank for each cell in the matrix is the product of the toxicity weight and the exposure weight for the row and column that define the cell. The ORD simplified approach to classifying toxic chemicals provides an example of values assigned to matrix cells. OTS's TSCA prescreening of TRI chemicals also presents an exposure/toxicity matrix, but assigns ranks of low, medium or high to each cell, rather than numerical weights.

**Step 6. Individual chemical-facility indices are derived for each medium by multiplying the rank for the cell in which the chemical falls, the population exposed via that medium, and the emissions to that medium.**

**Step 7. The overall index is the sum of the media-specific indices across all chemicals and across all facilities.** An example demonstrating Option 3 for the sample data set is found in Figure 3.

**Advantages** - This method avoids combining toxicity categories. It provides a simple but informative rank for each chemical based on a two-way classification scheme. The final index weightings are explicit and understandable.

**Disadvantages** - This approach assumes that all of the toxicity categories are of equal importance. In this approach, chemicals do not get specific exposure-toxicity ranks; only the categories to which they belong are ranked. The use of three broad categories within the scoring elements does not allow fine-scale differentiation among values for chemicals within a scoring element. This particular flaw would prevent us from distinguishing changes in chemicals with very high toxicities from changes in "border" chemicals with marginally high toxicities. Options to address this problem include (a) eliminating "border" chemicals from the index calculation; and (b) performing more explicit analysis on the "border" chemicals to evaluate how different the index would be if they switched into different categories.

### Figure 3. Example Calculation for Option 3 Ranking System

Step 1. From among the toxicity criteria of interest, choose the lowest dose for each chemical among all the categories. This is the limiting dose.

Chemical	Cancer	Chronic Toxicity Other Than Cancer			LIMITING DOSE
		Liver	Neurologic	Reproductive	(mg/kg-day)
	Risk-specific Dose at 1E-4 Risk Level (mg/kg-day) (1E-4/q*)	RfD (mg/kg-day)	RfD (mg/kg-day)	RfD (mg/kg-day)	
A	1E-05	1E-01			1E-05
B	1E-01		2E-01		1E-01
C	1E-04			2E-02	1E-04
D	3E-03	5E-02			3E-03
E	2E-05		5E-03		2E-05
F	2E-06			1E-03	2E-06

Step 2. Place chemicals into high, medium and low categories.

For this step, we need to develop criteria for what constitutes a high, medium, or low toxicity. For the purposes of this example, we assign the following values to these categories:

Category	Range
High	Dose < 1E-4
Medium	1E-4 < Dose < 1E-2
Low	1E-2 < Dose

Using these criteria, we classify the chemicals:

Chemical	LIMITING DOSE (mg/kg-day)	TOXICITY CATEGORY
A	1E-05	High
B	1E-01	Low
C	1E-04	Medium
D	3E-03	Medium
E	2E-05	High
F	2E-06	High

Step 3. Based on salient physicochemical properties, assign chemicals to high, medium and low exposure potential categories.

For this step, we must establish media-specific criteria for assigning chemicals to high, medium and low categories.

For the purposes of this example, we make the following assignments:

Exposure Medium	Criterion		
	Low	Medium	High
Air	photolysis < 1E-7	1E-6 < photolysis < 1E-4	1E-4 < photolysis
Drinking Water	solubility < 10	10 < solubility < 500	500 < solubility
Fish	BCF < 50	50 < BCF < 500	500 < BCF

Using these criteria, we classify the chemicals:

Chemical	Air	Drinking Water	Fish
A	High	High	Low
B	Low	High	Medium
C	High	Low	Medium
D	Medium	Low	High
E	Low	Low	Low
F	Low	Medium	Low

Step 4. Using the exposure and toxicity ranks, create a toxicity-exposure matrix for each medium.

Toxicity-Exposure Matrix

Toxicity	Air Exposure			Drinking Water Exposure			Fish Ingestion Exposure		
	Low	Medium	High	Low	Medium	High	Low	Medium	High
Low	B					B		B	
Medium		D	C	C	D			C	D
High	E,F		A	E	F	A	A,E,F		

Step 5. Assign values to each cell in the matrix.

For this step, ranks are assigned the following values:

Category	Exposure Rank	Toxicity Rank
High	0.4	5
Medium	0.2	3
Low	0.1	1

The value for the cell is the product of the toxicity times the exposure rank.

Toxicity-Exposure Matrix Values

Toxicity	Air Exposure			Drinking Water Exposure			Fish Ingestion Exposure		
	Low	Medium	High	Low	Medium	High	Low	Medium	High
Low	0.1					0.4		0.2	
Medium		0.6	1.2	0.3	0.6			0.6	1.2
High	0.5		2	0.5	1	2	0.5		

Step 6. Combine facility-specific emissions and population data to obtain media-specific chemical scores.

### EMISSION-EXPOSURE SCORES

(FOR AIR:)

Facility	Chemical	Air Emissions (lb/yr)	Population Exposed Via Air	Matrix Value	AIR SCORE
1	A	1000	3000	2	6.0E+06
	B	2000	3000	0.1	6.0E+05
	C	2000	3000	1.2	7.2E+06
	E	4000	3000	0.5	6.0E+06
2	C	3000	1000	1.2	3.6E+06
	D	4000	1000	0.6	2.4E+06
	F	10000	1000	0.5	5.0E+06
3	A	2000	2000	2	8.0E+06
	C	4000	2000	1.2	9.6E+06
	D	6000	2000	0.6	7.2E+06
	E	1000	2000	0.5	1.0E+06
	TOTAL:				5.7E+07

(FOR WATER:)

Facility	Chemical	Water Emissions (lb/yr)	Population Exposed Via Water	Drinking Water Matrix Value	Fish Matrix Value	Average Matrix Value	WATER SCORE
1	A	6000	500	2	0.5	1.3	3.8E+06
	B	4000	500	0.4	0.2	0.3	6.0E+05
	C	1000	500	0.3	0.6	0.5	2.3E+05
	E	3000	500	0.5	0.5	0.5	7.5E+05
2	C	1000	6000	0.3	0.6	0.5	2.7E+06
	D	5000	6000	0.6	1.2	0.9	2.7E+07
	F	2000	6000	1	0.5	0.8	9.0E+06
3	A	4000	2000	2	0.5	1.3	1.0E+07
	C	2000	2000	0.3	0.6	0.5	1.8E+06
	D	10000	2000	0.6	1.2	0.9	1.8E+07
	E	6000	2000	0.5	0.5	0.5	6.0E+06
	TOTAL:						8.0E+07

Step 7. Combine the media-specific ranks to obtain overall rank.

Facility	Chemical	AIR SCORE	WATER SCORE	OVERALL SCORE
1	A	6.0E+06	3.8E+06	9.8E+06
	B	6.0E+05	6.0E+05	1.2E+06
	C	7.2E+06	2.3E+05	7.4E+06
	E	6.0E+06	7.5E+05	6.7E+06
2	C	3.6E+06	2.7E+06	6.3E+06
	D	2.4E+06	2.7E+07	2.9E+07
	F	5.0E+06	9.0E+06	1.4E+07
3	A	8.0E+06	1.0E+07	1.8E+07
	C	9.6E+06	1.8E+06	1.1E+07
	D	7.2E+06	1.8E+07	2.5E+07
	E	1.0E+06	6.0E+06	7.0E+06
	TOTAL:	5.7E+07	8.0E+07	1.4E+08

## **Appendix C**

### **Available Toxicity Data for TRI Chemicals**

## Sorted Compilation of Toxicity Weights for Scored TRI Chemicals

Table C-1 contains all TRI chemicals on the 1995 roster which have been assigned toxicity weights, by sorted toxicity weight category.

Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight				
CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
Chemicals With One or More Toxicity Weights of 1,000,000				
92-87-5	Benzidine	1000000	1000000	IRIS
542-88-1	Bis(chloromethyl)ether	1000000	1000000	IRIS
106-93-4	Dibromoethane, 1,2-	10000	1000000	IRIS
77-78-1	Dimethyl sulfate	1000000	1000000*	interim derived
759-73-9	N-Nitroso-N-ethylurea	1000000*	1000000	HEAST
55-18-5	N-Nitrosodiethylamine	1000000	1000000	IRIS
62-75-9	N-Nitrosodimethylamine	100000	1000000	IRIS
75-55-8	Propyleneimine	1000000*	1000000	final derived
1314-20-1	Thorium dioxide	10000	1000000	final derived
Chemicals With One or More Toxicity Weights of 100,000				
107-02-8	Acrolein	100000	100000*	IRIS
309-00-2	Aldrin	100000	100000	IRIS
319-84-6	alpha-Hexachlorocyclohexane	100000	100000	IRIS
7429-90-5	Aluminum (fume or dust)	100000		interim derived
7440-38-2	Arsenic	100000	10000	IRIS
N020	Arsenic compounds	100000	10000	IRIS
98-07-7	Benzotrichloride	100000*	100000	IRIS
N050	Beryllium compounds	100000	10000	IRIS
7440-41-7	Beryllium	100000	10000	IRIS
56-35-9	Bis(tributyltin) oxide	100000*	100000	IRIS
2602-46-2	C.I. Direct Blue 6	100000*	100000	HEAST
1937-37-7	C.I. Direct Black 38	100000*	100000	HEAST

Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight				
CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
16071-86-6	C.I. Direct Brown 95	100000*	100000	HEAST
7440-43-9	Cadmium	100000	10000	IRIS
N078	Cadmium compounds	100000	10000	IRIS
532-27-4	Chloroacetophenone, 2-	100000	100000*	IRIS
7440-48-4	Cobalt	100000	100000*	interim derived
N096	Cobalt compounds	100000	100000*	interim derived
25376-45-8	Diaminotoluene (mixed isomers)	100000*	100000	interim derived
764-41-0	Dichloro-2-butene, 1,4-	100000	100000*	HEAST
119-93-7	Dimethylbenzidine, 3,3'-	100000*	100000	HEAST
302-01-2	Hydrazine	100000	10000	IRIS
78-84-2	Isobutyraldehyde	100000	100000*	interim derived
N420	Lead compounds	100000	100000	interim derived
7439-92-1	Lead	100000	100000	interim derived
109-77-3	Malonitrile	100000*	100000	HEAST
7439-96-5	Manganese	100000	10	IRIS
N450	Manganese compounds	100000	10	IRIS
150-50-5	Merphos	100000*	100000	IRIS
624-83-9	Methyl isocyanate	100000	100000*	final derived
924-16-3	N-Nitrosodi-n-butylamine	100000	100000	IRIS
621-64-7	N-Nitrosodi-n-propylamine	100000*	100000	IRIS
7723-14-0	Phosphorus (yellow or white)	100000*	100000	IRIS
N575	Polybrominated Biphenyls (PBBs)	100000*	100000	HEAST
1336-36-3	Polychlorinated biphenyls	1000	100000	IRIS
62-74-8	Sodium fluoroacetate	100000*	100000	IRIS
7550-45-0	Titanium tetrachloride	100000	100000*	interim derived
584-84-9	Toluene-2,4-diisocyanate	100000	100	final derived

Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight				
CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
91-08-7	Toluene-2,6-Diisocyanate	100000	100	final derived
26471-62-5	Toluenediisocyanate	100000	100	IRIS
78-48-8	Tributyltrithiophosphate (DEF), S,S,S-	100000*	100000	IRIS
Chemicals With One or More Toxicity Weights of 10,000				
79-06-1	Acrylamide	10000	10000	IRIS
79-10-7	Acrylic acid	10000	10	IRIS
107-13-1	Acrylonitrile	1000	10000	IRIS
107-05-1	Allyl chloride	10000	10000*	IRIS
20859-73-8	Aluminum phosphide	10000*	10000	IRIS
62-53-3	Aniline	10000	100	IRIS
7440-36-0	Antimony	10000*	10000	IRIS
N010	Antimony compounds	10000*	10000	IRIS
111-44-4	Bis(2-chloroethyl)ether	10000	10000	IRIS
106-99-0	Butadiene, 1,3-	10000	10000*	IRIS
141-32-2	Butyl acrylate	10	10000	interim derived
57-74-9	Chlordane	10000	10000	IRIS
10049-04-4	Chlorine dioxide	10000	10000*	IRIS
95-80-7	Diaminotoluene, 2,4-	10000*	10000	HEAST
96-12-8	Dibromo-3-chloropropane (DBCP), 1,2-	10000	10000*	IRIS
542-75-6	Dichloropropylene, 1,3-	100	10000	IRIS
62-73-7	Dichlorvos	10000	10000	IRIS
64-67-5	Diethyl sulfate	10000*	10000	final derived
60-51-5	Dimethoate	10000*	10000	IRIS
534-52-1	Dinitro-o-cresol, 4,6-	10000	10000	interim derived
606-20-2	Dinitrotoluene, 2,6-	10000*	10000	IRIS
122-66-7	Diphenylhydrazine, 1,2-	10000	10000	IRIS

**Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight**

CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
106-89-8	Epichlorohydrin	10000	100	IRIS
96-45-7	Ethylene thiourea	10000*	10000	IRIS
75-21-8	Ethylene oxide	10000*	10000	HEAST
76-44-8	Heptachlor	10000	10000	IRIS
118-74-1	Hexachlorobenzene	10000	10000	IRIS
70-30-4	Hexachlorophene	10000*	10000	IRIS
67485-29-4	Hydramethylnon (Tetrahydro-5,5-di-methyl-2(1H)- pyrimidinone[3-[4-(trifluoromethyl)phenyl]-1-[2-[4-(trifluoromet	10000*	10000	IRIS
7783-06-4	Hydrogen sulfide	10000	1000	IRIS
58-89-9	Lindane	10000*	10000	IRIS
99-65-0	m-Dinitrobenzene	10000*	10000	IRIS
7439-97-6	Mercury	10000	10000*	IRIS
N458	Mercury compounds	10000	10000*	IRIS
126-98-7	Methacryonitrile	10000*	10000	IRIS
94-74-6	Methoxone ((4-Chloro-2-methylphenoxy)acetic acid) (MCPA)	10000*	10000	IRIS
298-00-0	Methyl parathion	10000*	10000	IRIS
1313-27-5	Molybdenum trioxide	10000	1000	interim derived
98-95-3	Nitrobenzene	10000*	10000	IRIS
55-63-0	Nitroglycerin	10000*	10000	interim derived
90-04-0	o-Anisidine	10000	1000	interim derived
528-29-0	o-Dinitrobenzene	10000*	10000	HEAST
100-25-4	p-Dinitrobenzene	10000*	10000	HEAST
7803-51-2	Phosphine	10000	10000	IRIS
88-89-1	Picric acid	10000	10000	final derived
91-22-5	Quinoline	10000*	10000	HEAST
No CASRNb	Strychnine and salts	10000*	10000	IRIS

Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight				
CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
7664-93-9	Sulfuric acid	10,000	1	final derived
62-56-6	Thiourea	10000*	10000	final derived
8001-35-2	Toxaphene	10000	10000	IRIS
75-01-4	Vinyl chloride	10000*	10000	HEAST
81-81-2	Warfarin and salts	10000*	10000	IRIS
Chemicals With One or More Toxicity Weights of 1,000				
30560-19-1	Acephate (Acetylphosphoramidothioic acid O,S-dimethyl ester)	1000*	1000	IRIS
75-07-0	Acetaldehyde	1000	1000*	IRIS
116-06-3	Aldicarb	1000*	1000	IRIS
107-18-6	Allyl alcohol	1000*	1000	IRIS
33089-61-1	Amitraz	1000*	1000	IRIS
1332-21-4	Asbestos (friable)	1000	n/a	IRIS
100-44-7	Benzyl chloride	1000*	1000	IRIS
74-83-9	Bromomethane (Methyl Bromide)	1000	1000	IRIS
156-62-7	Calcium cyanamide	1000*	1000	final derived
1563-66-2	Carbofuran	1000*	1000	IRIS
56-23-5	Carbon tetrachloride	1000	1000	IRIS
79-11-8	Chloroacetic acid	1000*	1000	HEAST
67-66-3	Chloroform	1000	100	IRIS
80-15-9	Cumene hydroperoxide	1000	1000*	final derived
135-20-6	Cupferron	1000*	1000	final derived
68085-85-8	Cyhalothrin (3-(2-Chloro-3,3,3-trifluoro-1-propenyl)-2,2-Dimethylcyclopropanecarboxylic acidcyano(3-phenoxypheny	1000*	1000	IRIS
2303-16-4	Diallate	1000*	1000	HEAST
101-80-4	Diaminodiphenylether, 4,4'-	1000*	1000	final derived
91-94-1	Dichlorobenzidine, 3,3'-	1000*	1000	IRIS

Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight				
CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
75-27-4	Dichlorobromomethane	1000*	1000	IRIS
107-06-2	Dichloroethane, 1,2-	1000	1000	IRIS
120-83-2	Dichlorophenol, 2,4-	1000*	1000	IRIS
78-87-5	Dichloropropane, 1,2-	1000	1000*	IRIS
576-26-1	Dimethylphenol, 2,6-	1000*	1000	IRIS
88-85-7	Dinitrobutyl phenol (Dinoseb)	1000*	1000	IRIS
51-28-5	Dinitrophenol, 2,4-	1000*	1000	IRIS
121-14-2	Dinitrotoluene, 2,4-	1000*	1000	IRIS
330-54-1	Diuron	1000*	1000	IRIS
2439-10-3	Dodine (Dodecylguanidine monoacetate)	1000*	1000	IRIS
67-72-1	Hexachloroethane	10	1000	IRIS
74-90-8	Hydrogen cyanide	1000	100	IRIS
77501-63-4	Lactofen (5-(2-Chloro-4-(trifluoromethyl)phenoxy)-2-nitro-2-ethoxy-1-methyl-2-oxoethyl ester)	1000*	1000	IRIS
330-55-2	Linuron	1000*	1000	IRIS
12427-38-2	Maneb	1000*	1000	IRIS
93-65-2	Mecoprop	1000*	1000	IRIS
72-43-5	Methoxychlor	1000*	1000	IRIS
74-88-4	Methyl iodide	1000*	1000	interim derived
101-14-4	Methylenebis(2-chloroaniline), 4,4'-	1000	1000	HEAST
90-94-8	Michlers Ketone	1000*	1000	final derived
2212-67-1	Molinate (1H-Azepine-1 carbothioicacid, hexahydro-S-ethyl ester)	1000*	1000	IRIS
121-69-7	N,N-Dimethylaniline	1000*	1000	IRIS
300-76-5	Naled	1000*	1000	IRIS
100-02-7	Nitrophenol, 4-	1000	1000	final derived
95-53-4	o-Toluidine	1000*	1000	HEAST

**Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight**

CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
636-21-5	o-Toluidine hydrochloride	1000*	1000	HEAST
19666-30-9	Oxydiazon (3-[2,4-Dichloro-5-(1-methylethoxy)phenyl]-5-(1,1-dimethylethyl)-1,3,4-oxadiazol-2(3H)-one)	1000*	1000	IRIS
42874-03-3	Oxyfluorfen	1000*	1000	IRIS
106-47-8	p-Chloroaniline	1000*	1000	IRIS
120-71-8	p-Cresidine	1000*	1000	interim derived
106-44-5	p-Cresol	1000*	1000	HEAST
1910-42-5	Paraquat dichloride	1000*	1000	IRIS
87-86-5	Pentachlorophenol	1000*	1000	IRIS
79-21-0	Peracetic acid	1000	1000*	interim derived
7664-38-2	Phosphoric acid	1000	1	IRIS
7287-19-6	Prometryn (N,N'-Bis(1-methylethyl)-6-methylthio-1,3,5-triazine-2,4-diamine)	1000*	1000	IRIS
709-98-8	Propanil (N-(3,4-Dichlorophenyl)propanamide)	1000*	1000	IRIS
107-19-7	Propargyl alcohol	1000*	1000	IRIS
114-26-1	Propoxur	1000*	1000	IRIS
75-56-9	Propylene oxide	100	1000	IRIS
110-86-1	Pyridine	1000*	1000	IRIS
82-68-8	Quintozene	1000*	1000	IRIS
7782-49-2	Selenium	1000*	1000	IRIS
N725	Selenium compounds	1000*	1000	IRIS
7440-22-4	Silver	1000*	1000	IRIS
N740	Silver compounds	1000*	1000	IRIS
122-34-9	Simazine	1000*	1000	IRIS
26628-22-8	Sodium azide	1000*	1000	IRIS
137-26-8	Thiram	1000*	1000	IRIS
79-00-5	Trichloroethane, 1,1,2-	100	1000	IRIS

Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight				
CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
121-44-8	Triethylamine	1000	1000*	IRIS
95-63-6	Trimethylbenzene, 1,2,4	1000	1000	final derived
593-60-2	Vinyl bromide	1000	1000*	IRIS
75-35-4	Vinylidene chloride	100	1000	IRIS
Chemicals With One or More Toxicity Weights of 100				
94-82-6	2,4-DB	100*	100	IRIS
94-75-7	Acetic acid (2,4-D((2,4-dichlorophenoxy)))	100*	100	IRIS
75-05-8	Acetonitrile	100*	100	IRIS
62476-59-9	Acifluorfen, sodium salt [5-(2-Chloro-4-(trifluoromethyl)phenoxy)-2-nitrobenzoic acid, sodium salt]	100*	100	IRIS
15972-60-8	Alachlor	100*	100	IRIS
834-12-8	Ametryn (N-Ethyl-N'-(1-methylethyl)-6-(methylthio)-1,3,5,-triazine- 2,4 diamine)	100*	100	IRIS
7664-41-7	Ammonia	100	100*	IRIS
1912-24-9	Atrazine (6-Chloro-N-ethyl-N'-(1-methylethyl)-1,3,5,-triazine-2,4-diamine)	100*	100	IRIS
17804-35-2	Benomyl	100*	100	IRIS
71-43-2	Benzene	100	100	IRIS
82657-04-3	Bifenthrin	100*	100	IRIS
92-52-4	Biphenyl	100*	100	IRIS
75-25-2	Bromoform (Tribromomethane)	10	100	IRIS
1689-99-2	Bromoxynil octanoate (Octanoic acid,2,6-dibromo-4-cyanophenyl ester)	100*	100	IRIS
1689-84-5	Bromoxynil (3,5-Dibromo-4-hydroxybenzonitrile)	100*	100	IRIS
106-88-7	Butylene oxide, 1,2-	100	100*	IRIS
463-58-1	Carbonyl sulfide	100	100*	interim derived
120-80-9	Catechol	100	100	interim derived

Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight				
CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
133-90-4	Chloramben	100*	100	IRIS
90982-32-4	Chlorimuron ethyl (Ethyl-2-[[[(4-chloro-6-methoxyprimidin-2-yl)-carbonyl]-amino]sulfonyl]benzoate)	100*	100	IRIS
108-90-7	Chlorobenzene	100*	100	IRIS
510-15-6	Chlorobenzilate	100*	100	IRIS
1897-45-6	Chlorothalonil	100*	100	IRIS
64902-72-3	Chlorsulfuron (2-Chloro-N-[[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino]carbonyl]benzenesulfonamide)	100*	100	IRIS
98-82-8	Cumene	100*	100	IRIS
N106	Cyanide compounds	100*	100	IRIS
68359-37-5	Cyfluthrin (3-(2,2-Dichloroethenyl)-2,2-dimethylcyclopropanecarboxylic acid,cyano(4-fluoro-3-phenoxyphenyl)methy	100*	100	IRIS
1163-19-5	Decabromodiphenyl oxide	100*	100	IRIS
117-81-7	Di(2-ethylhexyl) phthalate	100*	100	IRIS
1918-00-9	Dicamba (3,6-Dichloro-2-methoxybenzoicacid)	100*	100	IRIS
541-73-1	Dichlorobenzene, 1,3-	10	100	interim derived
25321-22-6	Dichlorobenzene (mixed isomers)	10	100	interim derived
540-59-0	Dichloroethylene, 1,2-	100*	100	HEAST
75-09-2	Dichloromethane	10	100	IRIS
111-42-2	Diethanolamine	100*	100	interim derived
35367-38-5	Diflubenzuron	100*	100	IRIS
55290-64-7	Dimethipin (2,3,-Dihydro-5,6-dimethyl-1,4-dithiin 1,1,4,4-tetraoxide)	100*	100	IRIS
119-90-4	Dimethoxybenzidine, 3,3'-	100*	100	HEAST
105-67-9	Dimethylphenol, 2,4-	100*	100	IRIS
123-91-1	Dioxane, 1,4-	100*	100	IRIS

**Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight**

CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
957-51-7	Diphenamid	100*	100	IRIS
122-39-4	Diphenylamine	100*	100	IRIS
759-94-4	Ethyl dipropylthiocarbamate (EPTC)	100*	100	IRIS
140-88-5	Ethyl acrylate	100*	100	HEAST
39515-41-8	Fenpropathrin (2,2,3,3-Tetramethylcyclopropane carboxylic acid cyano(3-phenoxyphenyl)methylester)	100*	100	IRIS
51630-58-1	Fenvalerate (4-Chloro-alpha-(1-methylethyl)benzeneacetic acid cyano(3-phenoxyphenyl)methyl ester)	100*	100	IRIS
2164-17-2	Fluometuron	100*	100	IRIS
69409-94-5	Fluvalinate (N-[2-Chloro-4-(trifluoromethyl)phenyl]-DL-valine(+)-cyano (3-phenoxyphenyl)methyl ester)	100*	100	IRIS
72178-02-0	Fomesafen (5-(2-Chloro-4-(trifluoromethyl)phenoxy)-Nmethylsulfonyl)-2-nitrobenzamide)	100*	100	IRIS
50-00-0	Formaldehyde	100	10	IRIS
87-68-3	Hexachloro-1,3-butadiene	100	100	IRIS
77-47-4	Hexachlorocyclopentadiene	100*	100	IRIS
51235-04-2	Hexazinone	100*	100	IRIS
7647-01-0	Hydrochloric acid	100	100*	IRIS
123-31-9	Hydroquinone	100*	100	HEAST
35554-44-0	Imazalil (1-[2-(2,4-Dichlorophenyl)-2-(2-propenyloxy)ethyl]-1H-imidazole)	100*	100	IRIS
80-05-7	Isopropylidenediphenol, 4,4'-	100*	100	IRIS
108-39-4	m-Cresol	100*	100	IRIS
121-75-5	Malathion	100*	100	IRIS
109-86-4	Methoxyethanol, 2-	100	100*	IRIS
96-33-3	Methyl acrylate	100*	100	HEAST

**Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight**

CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
74-95-3	Methylene bromide	100*	100	HEAST
101-61-1	Methylenebis(N,N-dimethylbenzenamine), 4,4'-	100*	100	IRIS
21087-64-9	Metribuzin	100*	100	IRIS
88671-89-0	Myclobutanil (.alpha.-Butyl-.alpha.-(4-chlorophenyl)-1H-1,2,4-triazole-1-propanenitrile)	100*	100	IRIS
68-12-2	N,N-Dimethylformamide	100	100*	IRIS
7697-37-2	Nitric acid	100	100*	final derived
139-13-9	Nitrilotriacetic acid	100*	100	interim derived
99-59-2	Nitro-o-anisidine, 5-	100*	100	HEAST
99-55-8	Nitro-o-toluidine	100*	100	HEAST
79-46-9	Nitropropane, 2-	100	100*	IRIS
27314-13-2	Norflurazon (4-Chloro-5-(methylamino)-2-[3-(trifluoromethyl)phenyl]-3(2H)-pyridazinone)	100*	100	IRIS
95-48-7	o-Cresol	100*	100	IRIS
19044-88-3	Oryzalin (4-(Dipropylamino)-3,5-dinitrobenzenesulfonamide)	100*	100	IRIS
56-38-2	Parathion	100*	100	HEAST
40487-42-1	Pendimethalin (N-(1-Ethylpropyl)-3,4-dimethyl-2,6-dinitrobenzenamine)	100*	100	IRIS
52645-53-1	Permethrin (3-(2,2-Dichloroethenyl)-2,2-dimethylcyclopropanecarboxylic acid,(3-phenoxyphenyl)methyl ester)	100*	100	IRIS
108-45-2	Phenylenediamine, 1,3-	100*	100	IRIS
29232-93-7	Pirimiphos methyl (O-(2-(Diethylamino)-6-methyl-4-pyrimidinyl)-O,O-dimethylphosphorothioate)	100*	100	IRIS
1918-16-7	Propachlor (2-Chloro-N-(1-methylethyl)-N-phenylacetamide)	100*	100	IRIS
2312-35-8	Propargite	100*	100	IRIS

**Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight**

CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
60207-90-1	Propiconazole (1-[2-(2,4-Dichlorophenyl)-4-propyl-1,3-dioxolan-2-yl]-methyl-1H-1,2,4,-triazole)	100*	100	IRIS
76578-14-8	Quizalofop-ethyl (2-[4-[(6-Chloro-2-quinoxalinyloxy]phenoxy] propanoic acid ethyl ester)	100*	100	IRIS
10453-86-8	Resmethrin ([5-(Phenylmethyl)-3-furanyl]methyl 2,2-dimethyl-3-(2-methyl-1-propenyl)cyclopropanecarboxylate)	100*	100	IRIS
5902-51-2	Terbacil (5-Chloro-3-(1,1-dimethylethyl)-6-methyl- 2,4 (1H,3H)-pyrimidinedione)	100*	100	IRIS
630-20-6	Tetrachloroethane, 1,1,1,2-	10	100	IRIS
79-34-5	Tetrachloroethane, 1,1,2,2-	100	100	IRIS
127-18-4	Tetrachloroethylene (Perchloroethylene)	100*	100	IRIS
961-11-5	Tetrachlorvinphos	100*	100	IRIS
28249-77-6	Thiobencarb (Carbamic acid, diethylthio-, S-(p-chlorobenzyl))	100*	100	IRIS
43121-43-3	Triadimefon (1-(4-Chlorophenoxy)-3,3-dimethyl-1-(1H-1,2,4-triazol-1-yl)-2-butanone)	100*	100	IRIS
2303-17-5	Triallate	100*	100	IRIS
101200-48-0	Tribenuron methyl (2-(4-Methoxy-6-methyl-1,3,5-triazin-2-yl)-methylamino)carbonylamino)sulfonyl-, methyl ester)	100*	100	IRIS
120-82-1	Trichlorobenzene, 1,2,4-	100*	100	IRIS
88-06-2	Trichlorophenol, 2,4,6-	100	100	IRIS
96-18-4	Trichloropropane, 1,2,3-	100*	100	IRIS
1582-09-8	Trifluralin	100*	100	IRIS
7440-62-2	Vanadium (fume or dust)	100*	100	HEAST
50471-44-8	Vinclozolin (3-(3,5-Dichlorophenyl)-5-ethenyl-5-methyl-2,4-oxazolidinedione)	100*	100	IRIS
12122-67-7	Zineb	100*	100	IRIS

Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight				
CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
Chemicals With One or More Toxicity Weights of 10				
98-86-2	Acetophenone	10*	10	IRIS
120-12-7	Anthracene	10*	10	IRIS
N040	Barium compounds	10*	10	IRIS
7440-39-3	Barium	10*	10	IRIS
1861-40-1	Benfluralin (N-Butyl-N-ethyl-2,6-dinitro-4-(trifluoromethyl)benzenamine)	10*	10	IRIS
133-06-2	Captan	10*	10	IRIS
63-25-2	Carbaryl	10*	10	IRIS
75-15-0	Carbon disulfide	10	10	IRIS
5234-68-4	Carboxin (5,6-Dihydro-2-methyl-N-phenyl-1,4-oxathiin-3-carboxamide)	10*	10	IRIS
75-69-4	CFC-11	10*	10	IRIS
75-71-8	CFC-12	10*	10	IRIS
7782-50-5	Chlorine	10*	10	IRIS
74-87-3	Chloromethane	10	10	HEAST
84-74-2	Dibutyl phthalate	10*	10	IRIS
106-46-7	Dichlorobenzene, 1,4-	10	10*	IRIS
95-50-1	Dichlorobenzene, 1,2	10*	10	IRIS
110-80-5	Ethoxyethanol, 2-	10	10*	IRIS
100-41-4	Ethylbenzene	10	10	IRIS
7782-41-4	Fluorine	10*	10	IRIS
133-07-3	Folpet	10*	10	IRIS
108-31-6	Maleic anhydride	10*	10	IRIS
67-56-1	Methanol	10*	10	IRIS
80-62-6	Methyl methacrylate	10*	10	HEAST
78-93-3	Methyl ethyl ketone	10	1	IRIS

**Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight**

CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
108-10-1	Methyl isobutyl ketone	10*	10	HEAST
71-36-3	n-Butyl alcohol	10*	10	IRIS
110-54-3	n-Hexane	10	10*	IRIS
86-30-6	N-Nitrosodiphenylamine	10*	10	IRIS
106-50-3	p-Phenylenediamine	10*	10	HEAST
1918-02-1	Picloram	10*	10	IRIS
23950-58-5	Pronamide	10*	10	IRIS
74051-80-2	Sethoxydim (2-[1-(Ethoxyimino)butyl]-5-[2-(ethylthio)propyl]-3-hydroxyl-2-cyclohexen-1-one)	10*	10	IRIS
100-42-5	Styrene	10	10	IRIS
34014-18-1	Tebuthiuron (N-[5-(1,1-Dimethylethyl)-1,3,4-thiadiazol-2-yl]- N,N'-dimethylurea)	10*	10	IRIS
23564-05-8	Thiophanate-methyl	10*	10	IRIS
108-88-3	Toluene	10	10	IRIS
95-95-4	Trichlorophenol, 2,4,5-	10*	10	IRIS
108-05-4	Vinyl acetate	10	10*	IRIS
7440-66-6	Zinc (fume or dust)	10*	10	IRIS
Chemicals with Toxicity Weights of 1 for Both Exposure Pathways				
6484-52-2	Ammonium nitrate (solution)	1*	1	final derived
75-68-3	Chloro-1,1-difluoroethane, 1-	1	1*	IRIS
75-00-3	Chloroethane (Ethyl chloride)	1	1*	IRIS
7440-50-8	Copper	1*	1	HEAST
110-82-7	Cyclohexane	1	1*	interim derived
107-21-1	Ethylene glycol	1*	1	IRIS
74-85-1	Ethylene	1	1*	final derived
64-18-6	Formic acid	1*	1	HEAST
76-13-1	Freon 113	1*	1	IRIS

**Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight**

CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
108-38-3	m-Xylene	1*	1	HEAST
1634-04-4	Methyl tert-butyl ether	1	1*	IRIS
No CASRNa	Nitrate compounds (water dissociable)	1*	1	IRIS
95-47-6	o-Xylene	1*	1	HEAST
108-95-2	Phenol	1*	1	IRIS
90-43-7	Phenylphenol, 2-	1*	1	HEAST
85-44-9	Phthalic anhydride	1*	1	IRIS
115-07-1	Propylene (Propene)	1	1*	final derived
1330-20-7	Xylene (mixed isomers)	1*	1	IRIS
Chemicals with No Toxicity Weights				
71751412	Abamectin (Avermectin B1)			new chemical, not derived
60-35-5	Acetamide			low priority chemical
53-96-3	Acetylaminofluorene, 2-			low priority chemical
107119	Allylamine			new chemical, not derived
134-32-7	alpha-Naphthylamine			low priority chemical
1344-28-1	Aluminum oxide (fibrous forms)			new chemical, derived, not reviewed
82-28-0	Amino-2-methyl-anthraquinone, 1-			low priority chemical
117-79-3	Aminoanthraquinone, 2-			low priority chemical
60-09-3	Aminoazobenzene, 4-			low priority chemical
92-67-1	Aminodiphenyl, 4-			low priority chemical
61-82-5	Amitrole			new chemical, not derived
101053	Anilazine (4,6-Dichloro-N-(2-chlorophenyl)-1,3,5-triazin-2-amine)			new chemical, not derived
492-80-8	Auramine			low priority chemical
22781233	Bendiocarb (2,2-Dimethyl-1,3-benzodioxol-4-ol methylcarbamate)			new chemical, not derived
98-87-3	Benzal chloride			insufficient data

Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight				
CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
55-21-0	Benzamide			low priority chemical
98-88-4	Benzoyl chloride			insufficient data
94-36-0	Benzoyl Peroxide			insufficient data
91-59-8	beta-Naphthylamine			new chemical, not derived
57-57-8	beta-Propiolactone			low priority chemical
108-60-1	Bis(2-chloro-1-methethyl)ether			new chemical, not derived
111-91-1	Bis(2-chloroethoxy)methane			new chemical, not derived
7637072	Boron trifluoride			new chemical, not derived
10294345	Boron trichloride			new chemical, not derived
314409	Bromacil (5-Bromo-6-methyl-3-(1-methylpropyl)-2,4(1H,3H)-pyrimidinedione)			new chemical, not derived
53404196	Bromacil lithium salt (2,4(1H,3H)-Pyrimidinedione, 5-bromo-6-methyl-3 (1-methylpropyl), lithium salt)			new chemical, not derived
7726956	Bromine			new chemical, not derived
35691657	Bromo-1-(bromomethyl)-1,3-propanedicarbonitrile, 1-			new chemical, not derived
52517	Bromo-2-nitropropane-1,3-diol(Bronopol), 2-			new chemical, not derived
353-59-3	Bromochlorodifluoromethane (Halon 1			new chemical, derived, not reviewed
75-63-8	Bromotrifluoromethane (Halon 1301)			new chemical, not derived
357573	Brucine			new chemical, not derived
1929733	butoxyethyl ester, 2,4-D			new chemical, not derived
94804	butyl ester, 2,4-D			new chemical, not derived
123-72-8	Butyraldehyde			insufficient data
842-07-9	C.I. Solvent Yellow 14			low priority chemical
97-56-3	C.I. Solvent Yellow 3			low priority chemical
128-66-5	C.I. Vat Yellow 4			low priority chemical

Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight				
CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
989-38-8	C.I. Basic Red 1			low priority chemical
569-64-2	C.I. Basic Green 4			low priority chemical
3761-53-3	C.I. Food Red 5			low priority chemical
6459945	C.I. Acid Red 114			new chemical, not derived
81-88-9	C.I. Food Red 15			low priority chemical
2832-40-8	C.I. Disperse Yellow 3			low priority chemical
4680-78-8	C.I. Acid Green 3			low priority chemical
28407376	C.I. Direct Blue 218			new chemical, not derived
3118-97-6	C.I. Solvent Orange 7			low priority chemical
76-14-2	CFC 114			new chemical, not derived
76-15-3	CFC 115			new chemical, not derived
2439012	Chinomethionat (6-Methyl-1,3-dithiolo[4,5-b]quinoxalin-2-one)			new chemical, not derived
115286	Chlorendic acid			new chemical, not derived
75887	Chloro-1,1,1-trifluoroethane (HCFC-133a), 2-			new chemical, not derived
354-25-6	Chloro-1,1,2,2-tetrafluoroethane, 1-			new chemical, not derived
460355	Chloro-1,1,1-trifluoropropane(HCFC-253fb), 3-			new chemical, not derived
2837-89-0	Chloro-1,1,1,2-tetrafluoroethane, 2-			new chemical, not derived
563473	Chloro-2-methyl-1-propene, 3-			new chemical, not derived
4080313	Chloroallyl)-3,5,7-triaza-1-azoniaadamantane chloride, 1-(3-			new chemical, not derived
2971382	chlorocrotyl ester, 2,4-D			new chemical, not derived
74-45-6	Chlorodifluoromethane (HCFC-22)			new chemical, not derived
107-30-2	Chloromethyl methyl ether			insufficient data
N084	Chlorophenols			new chemical, not derived
76062	Chloropicrin			new chemical, not derived
126-99-8	Chloroprene			insufficient data

**Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight**

CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
542767	Chloropropionitrile, 3-			new chemical, not derived
63938-10-3	Chlorotetrafluoroethane			new chemical, not derived
75729	Chlorotrifluoromethane (CFC-13)			new chemical, not derived
5598130	Chlorpyrifos methyl (O,O-Dimethyl-O-(3,5,6-trichloro-2-pyridyl)phosphorothioate)			new chemical, not derived
7440-47-3	Chromium			insufficient data
N090	Chromium compounds			insufficient data
N100	Copper compounds			insufficient data
8001-58-9	Creosote, coal tar			new chemical, not derived
1319-77-3	Cresol (mixed isomers)			insufficient data
4170303	Crotonaldehyde			new chemical, not derived
21725462	Cyanazine			new chemical, not derived
1134232	Cycloate			new chemical, not derived
108930	Cyclohexanol			new chemical, not derived
28057489	d-trans-Allethrin [d-trans-Chrysanthemic acid of d-allethrine]			new chemical, not derived
533744	Dazomet (Tetrahydro-3,5-dimethyl-2H-1,3,5-thiadiazine-2-thione)			new chemical, not derived
53404607	Dazomet sodium salt (2H-1,3,5-Thiadiazine-2-thione, tetrahydro-3,5-dimethyl-, ion(1-), sodium)			new chemical, not derived
13684565	Desmedipham			new chemical, not derived
39156-41-7	Diaminoanisole sulfate, 2,4-			low priority chemical
615-05-4	Diaminoanisole, 2,4-			low priority chemical
333415	Diazinon			new chemical, not derived
334-88-3	Diazomethane			low priority chemical
132-64-9	Dibenzofuran			insufficient data
124-73-2	Dibromotetrafluoromethane (Halon 24)			new chemical, derived, not reviewed

**Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight**

CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
99309	Dichloran (2,6-Dichloro-4-nitroaniline)			new chemical, not derived
422560	Dichloro-1,1,1,2,2-pentafluoropropane (HCFC-225ca), 3,3-			new chemical, not derived
1649087	Dichloro-1,1-difluoroethane (HCFC-132b), 1,2-			new chemical, not derived
507551	Dichloro-1,1,2,2,3-pentafluoropropane (HCFC-225cb), 1,3-			new chemical, not derived
812-04-4	Dichloro-1,2,2-trifluoroethane (HCFC-123b), 1,1-			new chemical, not derived
111512562	Dichloro-1,2,3,3,3-pentafluoropropane (HCFC-225eb), 1,1-			new chemical, not derived
422480	Dichloro-1,1,1,2,3-pentafluoropropane (HCFC-225ba), 2,3-			new chemical, not derived
90454-18-5	Dichloro-1,1,2-trifluoroethane			insufficient data
136013791	Dichloro-1,1,2,3,3-pentafluoropropane (HCFC-225ea), 1,3-			new chemical, not derived
13474889	Dichloro-1,2,2,3,3-pentafluoropropane (HCFC-225cc), 1,1-			new chemical, not derived
431867	Dichloro-1,1,3,3,3-pentafluoropropane (HCFC-225da), 1,2-			new chemical, not derived
422446	Dichloro-1,1,2,3,3-pentafluoropropane (HCFC-225bb), 1,2-			new chemical, not derived
128903219	Dichloro-1,1,1,3,3-pentafluoropropane (HCFC-225aa), 2,2-			new chemical, not derived
354-23-4	Dichloro-1,1,2-trifluoroethane, 1,2-			new chemical, not derived
306-83-2	Dichloro-1,1,1-trifluoroethane, 2,2-			new chemical, not derived
1717-00-6	Dichloro-1-fluoroethane, 1,1-			new chemical, not derived
612839	Dichlorobenzidine dihydrochloride, 3,3'-			new chemical, not derived
64969342	Dichlorobenzidine sulfate, 3,3'-			new chemical, not derived
75434	Dichlorofluoromethane (HCFC-21)			new chemical, not derived
127564925	Dichloropentafluoropropane			new chemical, not derived
97234	Dichlorophene (2,2'-Methylenebis(4-chlorophenol))			new chemical, not derived

**Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight**

CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
78-88-6	Dichloropropene, 2,3-			new chemical, not derived
34077-87-7	Dichlorotrifluoroethane			new chemical, not derived
51338273	Diclofop methyl (2-[4-(2,4-Dichlorophenoxy)phenoxy]propanoic acid, methyl ester)			new chemical, not derived
115-32-2	Dicofol			low priority chemical
77736	Dicyclopentadiene			new chemical, not derived
1464-53-5	Diepoxybutane			low priority chemical
38727558	Diethyl ethyl			new chemical, not derived
101906	Diglycidyl resorcinol ether			new chemical, not derived
94-58-6	Dihydrosafrole			new chemical, not derived
No CASRN	Diisocyanates			new chemical, not derived
20325400	Dimethoxybenzidine dihydrochloride(o-Dianisidine dihydrochloride), 3,3'-			new chemical, not derived
111984099	Dimethoxybenzidine hydrochloride(o-Dianisidine hydrochloride), 3,3'-			new chemical, not derived
2524030	Dimethyl chlorothiophosphate			new chemical, not derived
57-14-7	Dimethyl Hydrazine, 1,1-			insufficient data
131-11-3	Dimethyl phthalate			insufficient data
2300665	Dimethylamine dicamba			new chemical, not derived
124403	Dimethylamine			new chemical, not derived
60-11-7	Dimethylaminoazobenzene, 4-			low priority chemical
612828	Dimethylbenzidine dihydrochloride(o-Tolidine dihydrochloride), 3,3'-			new chemical, not derived
41766750	Dimethylbenzidine dihydrofluoride(o-Tolidine dihydrofluoride), 3,3'-			new chemical, not derived
79-44-7	Dimethylcarbaryl chloride			low priority chemical
25321-14-6	Dinitrotoluene (mixed isomers)			new chemical, not derived
39300453	Dinocap			new chemical, not derived

**Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight**

CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
2164070	Dipotassium endothall (7-Oxabicyclo(2.2.1)heptane-2,3-dicarboxylic acid, dipotassium salt)			new chemical, not derived
136458	Dipropyl isocinchomeronate			new chemical, not derived
138932	Disodium cyanodithioimidocarbonate			new chemical, not derived
541537	Dithiobiuret, 2,4-			new chemical, not derived
120365	DP (Dichlorprop), 2,4-			new chemical, not derived
13194484	Ethoprop (Phosphorodithioic acid O-ethyl S,S-dipropyl ester)			new chemical, not derived
541-41-3	Ethyl chloroformate			low priority chemical
53404378	ethyl-4-methylpentyl ester, 2,4-D 2-			new chemical, not derived
N1000	Ethylenebisdithiocarbamic acid, salts and esters			insufficient data
151-56-4	Ethyleneimine (Aziridine)			low priority chemical
1928434	ethylhexyl ester, 2,4-D 2-			new chemical, not derived
75-34-3	Ethylidene dichloride			insufficient data
52857	Famphur			new chemical, not derived
60168889	Fenarimol (.alpha.-(2-Chlorophenyl)-.alpha.-4-chlorophenyl)-5-pyrimidinemethanol)			new chemical, not derived
13356086	Fenbutatin oxide (hexakis(2-methyl-2-phenylpropyl)distannoxane)			new chemical, not derived
66441234	Fenoxaprop ethyl (2-(4-((6-Chloro-2-benzoxazolylen)oxy)phenoxy)propanoic acid, ethyl ester)			new chemical, not derived
72490018	Fenoxycarb (2-(4-Phenoxyphenoxy)ethyl]carbamic acid ethyl ester)			new chemical, not derived
55389	Fenthion (O,O-Dimethyl O-[3-methyl-4-(methylthio) phenyl] ester, phosphorothioic acid)			new chemical, not derived
14484641	Ferbam (Tris(dimethylcarbamo dithioato-S,S')iron)			new chemical, not derived

**Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight**

CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
69806504	Fluazifop butyl (2-[4-[[5-(Trifluoromethyl)-2-pyridinyl]oxy]-phenoxy]propanoic acid, butyl ester)			new chemical, not derived
51218	Fluorouracil (5-Fluorouracil)			new chemical, not derived
N230	Glycol Ethers			insufficient data
1335-87-1	Hexachloronaphthalene			low priority chemical
680-31-9	Hexamethylphosphoramide			low priority chemical
10034-93-2	Hydrazine sulfate			insufficient data
7664-39-3	Hydrogen fluoride			insufficient data
55406536	Iodo-2-propynyl butylcarbamate, 3-			new chemical, not derived
13463406	Iron pentacarbonyl			new chemical, not derived
465736	Isodrin			new chemical, not derived
25311711	Isufenphos (2-[[Ethoxyl[(1-methylethyl)amino]phosphinothioyl]oxy]benzoic acid 1-methylethyl ester)			new chemical, not derived
94111	isopropyl ester, 2,4-D			new chemical, not derived
67-63-0	Isopropyl alcohol			interim derived
120-58-1	Isosafrole			new chemical, not derived
554132	Lithium carbonate			new chemical, not derived
149304	Mercaptobenzothiazole (MBT), 2-			new chemical, not derived
137428	Metham sodium (Sodiummethyldithiocarbamate)			new chemical, not derived
20354261	Methazole (2-(3,4-Dichlorophenyl)-4-methyl-1,2,4-oxadiazolidine-3,5-dione)			new chemical, not derived
2032657	Methiocarb			new chemical, not derived
3653483	Methoxone sodium salt ((4-Chloro-2-methylphenoxy) acetate sodium salt)			new chemical, not derived
556616	Methyl isothiocyanate			new chemical, not derived
60-34-4	Methyl hydrazine			insufficient data
74-93-1	Methyl mercaptan			new chemical, not derived

**Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight**

CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
79-22-1	Methyl chlorocarbonate			new chemical, not derived
101-77-9	Methylenedianiline, 4,4'-			insufficient data
75865	Methylactonitrile, 2-			new chemical, not derived
109-06-8	Methylpyridine, 2-			new chemical, not derived
75796	Methyltrichlorosilane			new chemical, not derived
9006422	Metiram			new chemical, not derived
7786347	Mevinphos			new chemical, not derived
150685	Monuron			new chemical, not derived
505-60-2	Mustard gas			low priority chemical
872504	N-Methyl-2-pyrrolidone			new chemical, not derived
924425	N-Methylolacrylamide			new chemical, not derived
684-93-5	N-Nitroso-N-methylurea			low priority chemical
4549-40-0	N-Nitrosomethylvinylamine			low priority chemical
59-89-2	N-Nitrosomorpholine			low priority chemical
16543-55-8	N-Nitrosornicotine			low priority chemical
100-75-4	N-Nitrosopiperidine			low priority chemical
142596	Nabam			new chemical, not derived
7440-02-0	Nickel			insufficient data
N495	Nickel compounds			insufficient data
No CASRN	Nicotine and salts			new chemical, not derived
1929824	Nitrapyrin (2-Chloro-6-(trichloromethyl)pyridine)			new chemical, not derived
92-93-3	Nitrobiphenyl, 4-			low priority chemical
1836-75-5	Nitrofen			low priority chemical
51-75-2	Nitrogen mustard			low priority chemical
88-75-5	Nitrophenol, 2-			insufficient data
134-29-2	o-Anisidine hydrochloride			low priority chemical

**Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight**

CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
2234-13-1	Octachloronaphtahlene			low priority chemical
20816-12-0	Osmium tetroxide			low priority chemical
301122	Oxydemeton methyl (S-(2-(Ethylsulfinyl)ethyl) O,O-dimethylester phosphorothioic acid)			new chemical, not derived
10028156	Ozone			new chemical, not derived
104-94-9	p-Anisidine			low priority chemical
95692	p-Chloro-o-toluidine			new chemical, not derived
104121	p-Chlorophenyl isocyanate			new chemical, not derived
100016	p-Nitroaniline			new chemical, not derived
156-10-5	p-Nitrosodiphenylamine			low priority chemical
123-67-7	Paraldehyde			new chemical, not derived
1114712	Pebulate (Butylethylcarbamothioic acidS-propyl ester)			new chemical, not derived
76-01-7	Pentachloroethane			new chemical, not derived
57330	Pentobarbital sodium			new chemical, not derived
594423	Perchloromethyl mercaptan			new chemical, not derived
85018	Phenanthrene			new chemical, not derived
26002802	Phenothrin (2,2-Dimethyl-3-(2-methyl-1-propenyl) cyclopropanecarboxylic acid(3-phenoxyphenyl)methyl ester)			new chemical, not derived
615281	Phenylenediamine dihydrochloride, 1,2-			new chemical, not derived
624180	Phenylenediamine dihydrochloride, 1,4-			new chemical, not derived
95545	Phenylenediamine, 1,2-			new chemical, not derived
57410	Phenytoin			new chemical, not derived
75-44-5	Phosgene			low priority chemical
51036	Piperonyl butoxide			new chemical, not derived
No CASRN	Polychlorinated alkanes			new chemical, not derived
No CASRN	Polycyclic aromatic compounds			new chemical, not derived

**Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight**

CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
7758012	Potassium bromate			new chemical, not derived
137417	Potassium N-methyldithiocarbamate			new chemical, not derived
128030	Potassium dimethyldithiocarbamate			new chemical, not derived
41198087	Profenofos (O-(4-Bromo-2-chlorophenyl)-O-ethyl-S-propyl phosphorothioate)			new chemical, not derived
1120-71-4	Propane sultone			new chemical, not derived
31218834	Propetamphos (3-[(Ethylamino)methoxyphosphinothioyl]oxy]-2-butenic acid, 1-methylethylester)			new chemical, not derived
123-38-6	Propionaldehyde			insufficient data
1320189	propylene glycol butyl etherester, 2,4-D			new chemical, not derived
106-51-4	Quinone			low priority chemical
81-07-2	Saccharin (manufacturing)			low priority chemical
94-59-7	Safrole			low priority chemical
78-92-2	sec-Butyl alcohol			insufficient data
2702729	sodium salt, 2,4-D			new chemical, not derived
132274	Sodium o-phenylphenoxide			new chemical, not derived
7632000	Sodium nitrite			new chemical, not derived
1982690	Sodium dicamba (3,6-Dichloro-2-methoxybenzoic acid, sodium salt)			new chemical, not derived
128041	Sodium dimethyldithiocarbamate			new chemical, not derived
131522	Sodium pentachlorophenate			new chemical, not derived
96-09-3	Styrene oxide			low priority chemical
2699798	Sulfuryl fluoride (Vikane)			new chemical, not derived
35400432	Sulprofos (O-Ethyl O-[4-(methylthio)phenyl]phosphorodithioicacid S propyl ester)			new chemical, not derived
3383968	Temephos			new chemical, not derived
75-65-0	tert-Butyl Alcohol			insufficient data

**Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight**

CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
354143	Tetrachloro-1-fluoroethane(HCFC-121), 1,1,2,2-			new chemical, not derived
354110	Tetrachloro-2-fluoroethane(HCFC-121a), 1,1,1,2-			new chemical, not derived
64755	Tetracycline hydrochloride			new chemical, not derived
7696120	Tetramethrin (2,2-Dimethyl-3-(2-methyl-1-propenyl) cyclopropanecarboxylic acid (1,3,4,5,6,7-hexahydro-1,3-dioxo-2			new chemical, not derived
7440-28-0	Thallium			insufficient data
N760	Thallium compounds			insufficient data
148798	Thiabendazole (2-(4-Thiazolyl)-1H-benzimidazole)			new chemical, not derived
62-55-5	Thioacetamide			low priority chemical
139-65-1	Thiodianiline, 4,4'-			low priority chemical
59669260	Thiodicarb			new chemical, not derived
23564069	Thiophanate ethyl ([1,2-Phenylenebis(iminocarbonothioyl)]biscarbamic acid diethyl ester)			new chemical, not derived
79196	Thiosemicarbazide			new chemical, not derived
10061026	trans-1,3-Dichloropropene			new chemical, not derived
110576	trans-1,4-Dichloro-2-butene			new chemical, not derived
68-76-8	Triaziquone			low priority chemical
2155706	Tributyltin methacrylate			new chemical, not derived
1983104	Tributyltin fluoride			new chemical, not derived
52-68-6	Trichlorfon			new chemical, not derived
76028	Trichloroacetyl chloride			new chemical, not derived
79-01-6	Trichloroethylene			insufficient data
57213691	Triclopyr triethylammonium salt			new chemical, not derived
26644462	Triforine (N,N'-[1,4-Piperazinediylbis-2,2,2-trichloroethylidene)]bisformamide)			new chemical, not derived
2655154	Trimethylphenyl methylcarbamate, 2,3,5-			new chemical, not derived

Table C-1. Toxicity Weights for all TRI Chemicals, by Toxicity Weight				
CAS Number	Chemical Name	Toxicity Weight		Source
		Inhalation	Oral	
76879	Triphenyltin hydroxide			new chemical, not derived
639587	Triphenyltin chloride			new chemical, not derived
126-72-7	Tris(2,3-dibromopropyl)phosphate			new chemical, not derived
72-57-1	Trypan blue			new chemical, not derived
51-79-6	Urethane (Ethyl Carbamate)			new chemical, not derived
87-62-7	Xylidine, 2,6-			low priority chemical
N982	Zinc Compounds			insufficient data

\*Toxicity weight is adopted from the other exposure pathway.

## **Appendix D**

### **Physicochemical Properties of Chemicals Included in the Indicators**

## Physicochemical Properties of Chemicals Included in the Indicators

The Toxics Release Inventory (TRI) model requires a database of physicochemical properties and destruction/removal efficiencies to predict the fate and transport of the 370 TRI chemicals. The physicochemical properties of interest include rates of chemical decay in air and water; organic carbon-water and octanol-water partition coefficients ( $K_{oc}$  and  $K_{ow}$ , respectively); water solubilities; bioconcentration factors; Henry's Law constants ( $K_H$ ); and molecular weights. To evaluate the effects of treatment and disposal, the model requires removal efficiencies for publicly owned treatment works (POTWs), within-POTW partitioning percentages among volatilization, biodegradation, and sorption to sludge, and incinerator destruction and removal efficiencies (DREs). Values for all of these parameters are included in a database called CHEMICAL.DB. The information in this database was originally documented in November, 1992. Since that time, better data have become available, particularly for POTW removal efficiencies and within-POTW partitioning percentages. The most significant new data sources are the Environmental Fate Data Base (Syracuse Research Corporation, 1995) and the RREL Treatability Database Version 5.0, maintained by the U.S. EPA Risk Reduction Engineering Laboratory (U.S. EPA, 1994).

This appendix describes the methods used to update CHEMICAL.DB and provides the sources for all of the data. The 370 TRI chemicals are divided among five tables, depending on the dominant source of the data or the primary method used to estimate parameter values if no data were available. This appendix also provides a summary of the resolution of certain TRI reporting issues which affect the exposure modeling.

## Update of Physicochemical and Destruction/Removal Efficiencies Data

### Table 1: Organic Chemicals

Table 1 contains data on 303 organic chemicals of the 370 TRI chemicals. Originally, values for six of the physicochemical parameters ( $\log(K_{ow})$ ,  $K_{oc}$ , water solubility, Henry's Law constant, molecular weight, and bioconcentration factor) were obtained from a dBase file called 313PROPB.dbf. This file, provided by the Exposure Assessment Branch, was created for an earlier project using TRI data. This file includes the references used for those values taken from the literature and the estimation method used for those values that were calculated. Additional values of molecular weights came from the CRC Handbook (CRC, 1990) and the Merck Index (Budavari, 1989). Note that throughout the tables, if a compound is infinitely soluble in water, a value of  $10^7$  mg/L was entered.

Air decay and water decay rates were estimated by arithmetically averaging the high and low first-order rate constants derived from the high and low half-lives reported in Howard et al. (1991). A full description of how the half-lives were obtained is given in the reference. A few additional water decay rates were obtained from the EPA database PIRANHA (U.S. EPA, 1991),

for chloramben, tetrachlorvinphos, trifluralin, chlorothalonil, and fluometuron. An air decay rate for trifluralin was also obtained from U.S. EPA (1991).

The POTW removal efficiencies and the within-POTW partitioning values were obtained from U.S. EPA, 1986. The portion of the chemical that neither partitions to air nor sludge nor escapes in POTW effluent is assumed to biodegrade.

The values for incinerator destruction/removal efficiencies (DREs) were difficult to obtain. Because the TRI model uses the incinerator DRE to estimate the fraction of the chemical fed to the incinerator that is released to the air, the DRE should be written as a percent of the incinerator feed. However, for organics, this methodology ignores the fact that chemicals of concern, such as dioxins, may be formed during the incineration process. We assume that the typical municipal waste combustor destruction/removal efficiency for organics is 99 percent. The exceptions to this rule are PCBs, which are assumed to have a DRE of 99.9999 percent, as required by TSCA regulation.

Many data on  $\log(K_{ow})$ , water solubility, hydrolysis half-lives, Henry's Law constants, POTW removal efficiencies, and within-POTW partitioning values were updated with values from the Environmental Fate Data Base (Syracuse Research Corporation, 1995). These values were provided by David Lynch of the Exposure Assessment Branch. This database also includes values for vapor pressure but these data were not used for this analysis. The database file includes references for those data taken from the literature and the method used for those values that were estimated.

For this analysis, two modifications to the data in the Environmental Fate Data Base were necessary. First, the hydrolysis half-lives were converted to rates by assuming first-order decay. Secondly, the within-POTW partitioning values were converted to percentages of the total POTW removal efficiency before incorporation into CHEMICAL.DB. For example, if ten percent of a particular chemical volatilized, 20 percent biodegraded, 40 percent sorbed to sludge, and 30 percent was in the POTW effluent, the first three percentages were scaled to sum to 100 percent of the total POTW removal efficiency of 70 percent. Thus, in CHEMICAL.DB for this example, 14 percent (10/70) of the total removal efficiency would be attributed to volatilization, 29 percent (20/70) would be attributed to biodegradation, and 57 percent would be attributed to sorption to sludge.

Additional values of  $K_{oc}$  and bioconcentration factors were estimated using regression equations in Lyman et al. (1990). If solubility values were available, the following equation (Eq. 4-5 in the reference) was used to estimate  $K_{oc}$  values:

$$\log(K_{oc}) = -0.55 \log(S) + 3.64$$

Note that in this equation, solubility ( $S$ ) must be entered in units of milligrams per liter (mg/L). If only  $\log(K_{ow})$  data were available, Eq. 4-8 in the reference was used:

$$\log(K_{oc}) = 0.544 \log(K_{ow}) + 1.377$$

To predict bioconcentration factors, Eq. 5-2 in the reference, which requires  $\log(K_{ow})$  values, was used:

$$\log BCF = 0.76 \log(K_{ow}) - 0.23$$

For limitations on the range of values of dependent variables appropriate for these equations, the reader is referred to Lyman et al., 1990.

## **Table 2: Inorganic Chemicals**

Table 2 contains data on 36 inorganic chemicals and classes of inorganic chemicals. Classes of inorganic compounds are assumed to behave like the elemental inorganic compound. Because inorganics do not decay in air or water, or appreciably sorb to organic carbon, values for these parameters are assumed to be zero. Except for ammonia, values for within-POTW partitioning to volatilization and biodegradation are also assumed to be zero, and therefore the partitioning percentage to sludge is 100 percent for 35 compounds. Given that ammonia can be a gaseous or aqueous species, it was not possible to predict within-POTW partitioning percentages for this chemical. The Henry's Law constant for ammonia was estimated from stability constants presented in Morel, 1983.

BCF values for these inorganics were predominantly obtained from the dBase file described above, 313PROPB.dbf, with five exceptions: aluminum (U.S. EPA, 1988a); antimony (U.S. EPA, 1988b); cobalt (Jørgensen and Johnsen, 1981); silver (U.S. EPA, 1987); and, thallium (Tetra Tech, 1985).

It is impossible to accurately predict metal solubility without knowing the concentrations of other metal ions and ligands in the water. Currently, water solubilities of zero are entered for all inorganics except copper, ammonia, and phosphorus. The solubility of phosphorus (yellow or white) is from Merck (Budavari, 1989). A more realistic estimate of metal solubility could be obtained by assuming particular water characteristics, such as pH and major ligand concentrations, and estimating the concentrations of complexed metals, which would remain dissolved in the water and potentially bioavailable. At this time, however, water solubilities of inorganic compounds are not used for any modeling purposes in the TRI model.

POTW removal efficiencies were available from the RREL Treatability Database maintained by the U.S. EPA Risk Reduction Engineering Laboratory. This database was also supplied by David Lynch of the Exposure Assessment Branch. For any given chemical, the RREL Treatability Database provides a list of removal efficiencies published in the scientific literature. Each value is characterized by the technology used, the type of influent, and the scale of the experiment. For all values associated with activated sediment and full scale experiments, a geometric mean was derived and used as the POTW removal efficiency. The RREL Treatability Database did not provide within-POTW partitioning values, and therefore the default partitioning value of 100 percent to sludge was used (except for ammonia), as discussed above.

Another physicochemical property required to model the fate and transport of inorganic compounds is the soil-water partition coefficient,  $K_d$ .  $K_d$  values are needed to estimate leachate concentrations from landfills. For all the metals in Table 2, except aluminum, we used  $K_d$  values measured in column studies by Gerritse et al. (1982) for sand with an  $f_{oc}$  value of 0.0355 g/g, a cation exchange capacity of 0.22 meq/g, zero

clay content, and a solution pH of 5. (The assumption that the waste in landfills is like sand yields a conservative estimate of leachate concentration, because the low clay content and the relatively low pH will tend to increase movement of metals.) The median of the range of  $K_d$  values for each metal was taken, assuming a log-normal distribution. The same values were used for classes of inorganic compounds as for the elemental inorganic compound. For aluminum, the  $K_d$  value is based on Langmuir isotherm data presented in Bodek et al., 1988.

For incinerator destruction/removal efficiencies, values were taken from multiple hearth sludge incinerator studies, as reported in U.S. EPA, 1992.

**Table 3: Chemicals Missing POTW Removal Efficiencies**

Table 3 shows the three TRI chemicals for which POTW removal efficiencies and within-POTW partitioning percentages were not available. To derive POTW removal efficiencies and within-POTW partitioning percentages, we first categorized the chemicals for which values were available (from Table 1) into chemical classes; we then derived average values for these parameters for each chemical class. The average class values were then applied to chemical class members with no data. Chemicals were divided into nine classes based on their  $K_{ow}$  and  $K_H$  values (U.S. EPA, 1986):

$K_{ow} \leq 100, K_H < 10^{-3} \text{ atm} \cdot \text{m}^3/\text{mol}$   
 $K_{ow} \leq 100, 10^{-3} \leq K_H < 10^{-2} \text{ atm} \cdot \text{m}^3/\text{mol}$   
 $K_{ow} \leq 100, K_H > 10^{-2} \text{ atm} \cdot \text{m}^3/\text{mol}$   
 $100 < K_{ow} \leq 10,000, K_H < 10^{-3} \text{ atm} \cdot \text{m}^3/\text{mol}$   
 $100 < K_{ow} \leq 10,000, 10^{-3} \leq K_H < 10^{-2} \text{ atm} \cdot \text{m}^3/\text{mol}$   
 $100 < K_{ow} \leq 10,000, K_H > 10^{-2} \text{ atm} \cdot \text{m}^3/\text{mol}$   
 $K_{ow} > 10,000, K_H < 10^{-3} \text{ atm} \cdot \text{m}^3/\text{mol}$   
 $K_{ow} > 10,000, 10^{-3} \leq K_H < 10^{-2} \text{ atm} \cdot \text{m}^3/\text{mol}$   
 $K_{ow} > 10,000, K_H > 10^{-2} \text{ atm} \cdot \text{m}^3/\text{mol}$

The POTW removal efficiency values, percent volatilization values, and average sludge partitioning percentages were averaged for the chemicals within each class. (The percent that biodegrades is calculated by subtracting the percent that volatilizes and the percent that partitions to sludge from 100 percent). The chemicals lacking these values were divided into the same classes using the same  $K_{ow}$  and  $K_H$  criteria; the average class values were then assigned to these chemicals based on the class into which they fell.

**Table 4: Chemicals Missing Some Physicochemical and Removal Efficiencies Data**

Table 4 shows the two TRI chemical groups without data from the Environmental Fate Data Base or RREL Treatability Database.

Chlorophenols: Because 2-chlorophenol is a priority pollutant, we used available water solubility,  $K_{ow}$ , and  $K_{oc}$  data (Mabey et al., 1982) for that compound to represent the class. A  $K_H$  value was estimated based on the methods of Hine and Mookerjee (1975). POTW removal

efficiencies and partitioning percentages were then obtained by placing chlorophenols in the appropriate  $K_{ow}$  and  $K_H$  class, as described above.

Cyanide compounds: According to Bodek et al. (1988), hydrogen cyanide “is believed to be the most toxic component of cyanide solutions.” Therefore, solubility and  $K_H$  data for HCN are provided in Table 4. Sorption of HCN is fairly weak, so no  $K_{oc}$  or  $K_{ow}$  values were available; thus removal efficiencies or partitioning percentages could not be estimated.

### **Table 5: Chemicals Missing Significant Amounts of Data**

Table 5 presents the 25 chemicals for which the least information was found. Sources for data are as described for Table 1. Solubilities for ammonium sulfate, hydrogen sulfide, molybdenum trioxide, paraldehyde, and thorium dioxide were obtained from the Merck Index (Budavari, 1989). The 26 chemicals were not included in the Environmental Fate Data Base; if they were included in the RREL Treatability Database, there was insufficient information to estimate POTW removal efficiencies and partitioning percentages.

### **Summary of Resolution of Certain TRI Reporting Issues**

In March 1996, several reporting issues pertaining to the TRI chemicals ammonia, ammonium sulfate, and mineral acids were resolved. These issues and the corresponding agreed modifications or recommendations are summarized below.

#### **Ammonia and Ammonium Sulfate**

Effective for the 1994 reporting year, only the ammonia or a fraction of the water-dissociable portion of ammonia in a compound will be reportable to TRI. This includes anhydrous ammonia, aqueous ammonia, and ammonia from water-dissociable ammonium salts and other sources (the latter includes ammonium sulfate). The total quantity of ammonia is calculated, but only 10% of this counts towards threshold levels for reporting and it is this 10% which is actually reported. To re-calculate the original quantity of ammonia, one must multiply the reported quantity of releases and transfers (e.g., POTW) to water and land by 10 (air emissions are reported at 100%).

In order to make the ammonium sulfate reporting from 1988 to 1994 (erroneous reports will be accepted for 1994) comparable to the reporting change that will occur in 1994, the Indicators will calculate the ammonia fraction of this chemical and this reporting will be combined with ammonia reporting (and will use the toxicity ranking for ammonia) for these years. Ammonium sulfate will not appear in the Indicators. Releases and transfers to air will be multiplied by 0.273 (ammonium sulfate has a molecular weight of 132 g, of which 36 g are ammonia). All 1988-1994 releases and transfers of ammonium sulfate to water or land will be multiplied by the factor 0.0273. This will permit cross-year comparisons of this modified ammonia listing.

For all years, the unmodeled pounds will reflect exactly what is reported under TRI (i.e., 10% of water and land emissions). However, the modeled pounds and all other modeled analyses will use a 10X multiplier for releases/transfers to water and land (air emissions are already accurately reflected in reporting) beginning

in 1994 (this multiplier will also need to be used for modeled pounds of ammonium sulfate, i.e., wherever the factor of 0.0273 was used - this does not apply to ammonia reporting from 1988-1993).

### **Mineral Acids**

This includes sulfuric and hydrochloric acid. The Agency has made the decision to modify reporting to include only the more highly toxic exposures to aerosol releases of certain of these acids. The acid aerosols include mists, vapors, gas, fog and other airborne forms of any particle size. For sulfuric acid, this change in reporting takes place in 1994, while for hydrochloric acid the change takes place for reporting year 1995. The very high decay rate in water of these acids will greatly reduce any risk-based impacts associated with releases or transfers to water.

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Table 1: Organic Chemicals															
CAS Number	Chemical	Air Decay (hr <sup>-1</sup> )	Koc (mL/g)	H2O Decay (hr <sup>-1</sup> )	LOGKow	Kd (L/kg)	Water Solubility (mg/L)	POTW Partition (Removal)	POTW Partition (Sludge)	POTW Partition (Volat)	POTW Partition (Biod)	Incinerator DRE	BCF (L/kg)	Henry's (atm-m <sup>3</sup> /mol)	Molecular Weight
100027	4-Nitrophenol	0.114188095	236	0.021105443	1.91		16000	99.48	0.42219541616	92.390430237	7.1773220748	99	79	0.415	139
100254	p-Dinitrobenzene		143		1.46		500	45.75	2.55737704918	0	97.442622951	99	7.6	0	168.11
100414	Ethylbenzene	0.044536326	250	0.006257579	3.15		206	89.8	3.93095768374	38.240534521	57.817371938	99	15	0.00788	106
100425	Styrene	0.432557601	920	0.001547204	2.95		320	94.89	2.11824217515	8.2727368532	89.609020972	99	13.5	0.00275	104
100447	Benzyl chloride	0.017343132	139	0.04621	2.3		525	78.03	1.38408304498	6.4334230424	92.169678329	99	33	0.000412	127
100754	N-Nitrosopiperidine	0.153104799	9	0.155573034	0.36		76480	45.46	2.39771227453	0.065992081	97.558293005	99	1.1	0	350.27
101144	4,4'-Methylenebis (2-chloroaniline)	1.31458948	8000	0.011378973	3.91		13.9	81.57	20.6448449185	0	79.355155082	99	575	0	267.16
101611	4,4'-Methylenebis (N,N-dimethylbenzenamine)	1.906154747	9140	0.013309681	4.37		1.3	92.73	31.7373018441	0	68.251914159	99	2400	0	254
101688	Methylenebis(phenylisocyanate)	0.65729474	16470	0.0693147	5.22			99.99	3.1803180318	0	96.829682968	99	5460	0	250
101779	4,4'-Methylenedianiline	1.411966479	98	0.016503504	1.59		1000	75.38	0.95516052003	0	99.04483948	99	9.5	0	198
101804	4,4'-Diaminodiphenylether	1.270769831	315	0.005653654	2.22		139	76.37	1.34869713238	0	98.651302868	99	22	0	200
103231	Bis(2-ethylhexyl)adipate	0.146627288	15500	0.018566442	8.12		0.1	99.93	38.2567797458	0	61.743220254	99	2260	0	370
104949	p-Anisidine	0.719303678	17	0.006069798	0.95		24706	92.09	0.38006298187	0	99.609078076	99	3.1	0	123.15
105679	2,4-Dimethylphenol	0.320362142	18	0.016503504	2.3		7870	76.63	1.46156857628	0.052198878	98.499282265	99	150	0	122
106423	p-Xylene	0.090769274	260	0.002578673	3.15		162.4	96.12	2.97544735747	15.574282147	81.450270495	99	15	0.00753	106
106445	p-Cresol	0.254153966	49	0.36823444	1.94		21520	92.34	0.56313623565	0.010829543	99.436863764	99	17.6	0	108
106467	1,4-Dichlorobenzene	0.00190045	600	0.00059596	3.44		81.3	75.34	9.848685957	32.505972923	57.64534112	99	214	0.0024	147
106503	p-Phenylenediamine	1.361539105	13	0.011695528	-0.3		37000	45.43	2.37728373322	0	97.60070438	99	1	0	108
106514	Quinone	0.57762265	26	0.349461704	0.2		11130	51.81	1.91082802548	21.250723798	76.838448176	99	0.84	0.000479	108.09
106887	1,2-Butylene oxide	0.012499375	8	0.003180917	0.86		95000	75.95	0.81632653061	3.5418038183	95.641869651	99	1	0.00018	72
106898	Epichlorohydrin	0.0026115	10	0.003522	0.45		65900	46.05	2.34527687296	2.1715526602	95.504885993	99	1.2	0.00003	92
106934	1,2-Dibromoethane	0.00148355	98	0.00059596	1.96		4152	54.38	2.24347186466	25.78153733	71.974990805	99	10	0.000667	188
106990	1,3-Butadiene	0.500450394	116	0.002578673	1.99		735	97.32	0.50349362926	85.665844636	13.830661734	99	19.16	0.0736	54
107028	Acrolein	0.112217492	5	0.002578673	-0.01		212500	92.18	0.35799522673	1.008895639	98.622260794	99	344	0.000122	56
107051	Allyl chloride	0.126414528	50	0.015444	1.93		3370	84.36	0.82977714557	81.86344239	17.306780465	99	7.45	0.011	76.53
107062	1,2-Dichloroethane	0.00130571	32	0.00022463	1.48		8608	58.03	1.68878166466	37.342753748	60.968464587	99	2	0.00118	99
107131	Acrylonitrile	0.027697423	9	0.012180304	0.25		74500	92.19	0.3579563944	1.1172578371	98.513938605	99	48	0.000138	53
107186	Allyl alcohol	0.17	1.47	0.017	0.17			92.07	0.36928424025	0.054306506	99.587270555	99		0	58
107211	Ethylene glycol	0.04593144	4	0.008423664	-1.36		1000000	92.06	0.35846187269	0	99.630675646	99	10	0	62
107302	Chloromethyl methyl ether	0.016794315	36	23.10491	0.32			100	0	0.01	99.98	99	1	0.000304	80.51
108054	Vinyl acetate		19	0.003956	0.73		20000	92.4	0.36796536797	3.0735930736	96.558441558	99	2	0.000511	86

Table 1: Organic Chemicals

CAS Number	Chemical	Air Decay (hr <sup>-1</sup> )	Koc (mL/g)	H2O Decay (hr <sup>-1</sup> )	LOGKow	Kd (L/kg)	Water Solubility (mg/L)	POTW Partition (Removal)	POTW Partition (Sludge)	POTW Partition (Volat)	POTW Partition (Biod)	Incinerator DRE	BCF (L/kg)	Henry's (atm-m <sup>3</sup> /mol)	Molecular Weight
108101	Methyl isobutyl ketone	0.082959087	19	0.016503504	1.31		19000	92.25	0.40108401084	1.1165311653	98.482384824	99	2.4	0.000138	100
108316	Maleic anhydride		181	69.31472	1.62			100	0	0	100	99	10	0	98
108383	m-Xylene	0.146627288	166	0.002578673	3.2		161	96.25	3.25194805195	14.379220779	82.379220779	99	15	0.00718	106
108394	m-Cresol	0.345737129	34.6	0.007718234	1.96		22700	92.35	0.56307525717	0.01082837	99.426096373	99	20	0	108
108601	Bis(2-chloro-1-methethyl)ether	0.082696518	73	0.00088248	2.48		1700	50.47	3.86368139489	6.2017039826	89.934614623	99	9.3	0.000112	171
108883	Toluene	0.037989797	95	0.004266531	2.73		526	94.96	1.43218197136	18.260320135	80.318028644	99	37	0.00664	92
108907	Chlorobenzene	0.00522951	275	0.00030863	2.84		497.9	85.32	2.47304266292	28.633380216	68.893577121	99	447	0.00377	112
108952	Phenol	0.167206557	16	0.071525289	1.46		82800	92.15	0.42322300597	0	99.576776994	99	39	0	94
109068	2-Methylpyridine		9.6		1.11		10000000	92.11	0.39083704267	0.097709261	99.511453697	99	4.1	0	93.13
109773	Malonitrile		6.6	0.001375	-0.6		133000	45.42	2.37780713342	0	97.622192867	99	0.21	0	66.06
109864	2-Methoxyethanol	0.066882623	9	0.002578673	-0.77		1000000	92.06	0.35846187269	0.010862481	99.630675646	99	0.2	0	76
110805	2-Ethoxyethanol	0.071258121	21	0.002578673	-0.32		1000000	92.06	0.35846187269	0.010862481	99.630675646	99	0.5	0	90
110827	Cyclohexane	0.043819649	482	0.00059596	3.44		55	88.74	6.98670272707	9.139057922	83.88508226	99	242	0.0015	84
110861	Pyridine	0.00297752	5	0.016503504	0.65		1000000	92.09	0.36920403953	0.1085894234	99.511347595	99	2	0.00001	79
111422	Diethanolamine	0.52948743	4	0.026130548	-1.43		1000000	92.06	0.35846187269	0	99.630675646	99	0.05	0	105
111444	Bis(2-chloroethyl)ether	0.039505798	79	0.00059596	1.29		17200	22.77	6.58761528327	3.3816425121	90.030742205	99	11	0.00002	143
111911	Bis(2-chloroethoxy)methane		31	0.0000693	1.3		8100	22.57	6.69029685423	2.2596366859	91.05006646	99	5.7	0.00001	173.1
1120714	Propane sultone	0.096027947	2.04	0.081547	-0.28		1140000	70.61	0.9347117972	0.0708115	99.008639003	99	0.24	0	112.14
114261	Propoxur	0.536944999	160	0.001805	1.52		1859	92.17	0.43398068786	0	99.555169795	99	8.41	0	209.24
115071	Propylene (Propene)	0.22916416	219	0.002578673	1.77		200	98.91	0.38418764533	90.830047518	8.7958750379	99	13.18	0.196	42.08
115322	Dicofol		46900		5.02		1.32	98.37	45.2678662194	0	54.732133781	99	13900	0	370.47
1163195	Decabromodiphenyl ether	0.00103325	37530	0.00011979	12.11		0.02	99.07	62.4709801151	0	37.518926012	99		0	959.17
117793	2-Aminoanthraquinone	0.165752587	11800	0.006069798	2.43		0.16	48.36	3.90818858561	0	96.091811414	99	1720	0	223
117817	Di(2-ethylhexyl) phthalate	0.131458948	87420	0.003518247	7.6		0.34	99.93	38.2467727409	0	61.753227259	99	114	0.00001	390
118741	Hexachlorobenzene	0.0001016	14100	0.0000218	5.73		0.0062	98.43	60.6319211622	0.4571776897	38.910901148	99	14500	0.0017	285
119904	3,3'-Dimethoxybenzidine	1.098648269	230	0.011307308	1.81		60	46.15	2.77356446371	0	97.226435536	99	14.12	1.8e-13	254.43
119937	3,3'-Dimethylbenzidine	1.427831271	447	0.016503504	2.34		1300	76.76	1.51120375195	0	98.488796248	99	35.48	0	212.28
120127	Anthracene	0.801407491	16000	0.801407491	4.45		0.0434	94.15	33.4466277217	2.1879978757	64.365374403	99	675	0.00072	178
120581	Isosafrole	0.32	540	0.0026	3.37			64.08	11.1735330836	0.1872659176	88.639200999	99	72	0	162.18
120718	p-Cresidine	1.31458948	42	0.005634289	1.74		4721	46.05	2.71444082519	0	97.263843648	99	10	0	137.18
120809	Catechol	0.146627288	118	0.016503504	0.88		461400	92.08	0.38010425717	0	99.619895743	99	3	0	110
120821	1,2,4-Trichlorobenzene	0.00296909	1430	0.00059596	4.02		49	86.46	22.1952347907	9.5998149433	68.216516308	99	1202	0.00142	181

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120832	2,4-Dichlorophenol	0.017982592	126	0.548741518	3.06		4500	94.76	2.62769100886	0.021105952	97.340650063	99	100	0	163
121142	2,4-Dinitrotoluene	0.08664	201	0.01612	1.98		270	46.5	2.94623655914	0	97.032258065	99	19	0	182
12122677	Zineb		1230	0.693147	0.17		10	97.61	0.1331830755	0	99.866816925	99	170	0	275.73
121697	N,N-Dimethylaniline	0.144864093	80	0.018137219	2.31		1454	48.68	3.45110928513	3.5332785538	92.995069844	99	10	0.00006	121.18
122667	1,2-Diphenylhydrazine	1.270769831	947	0.03	2.94		68	54.01	6.62840214775	0	93.371597852	99	100	0	184
123319	Hydroquinone	0.146576216	9.3	0.906607412	0.59		72000	92.07	0.36928424025	0	99.63071576	99	39.8	0	110
123386	Propionaldehyde	0.11552453	4	0.016503504	0.59		306000	92.15	0.36896364623	0.6619641888	98.969072165	99	1.66	0.00007	58.08
123728	Butyraldehyde	0.13615391	9.4	0.016503504	0.88		71000	92.2	0.37960954447	0.9652928416	98.655097614	99	2.75	0.000115	72
123911	1,4-Dioxane	0.047065549	17	0.001598777	-0.27		1000000	45.53	2.37206237646	0.3514166484	97.254557435	99	0.4	0	88
124732	1,2-Dibromotetrafluoroethane		1202	0.14	2.96			98.48	2.38627132413	96.303818034	1.3099106418	99	141.3	0.162	260
126727	Tris (2,3-dibromopropyl)phosphate	0.397115572	1390	0.016503504	4.29		8	99.5	14.3819095477	0.040201005	85.577889447	99	2.75	0.00002	697.61
126987	Methacrylonitrile		16.5		0.68		25400	76.17	0.80084022581	4.5949849022	94.591046344	99	1.9	0.000247	67.09
126998	Chloroprene	0.13197481	312	0.00059596	2.53		480	95.71	1.1597534218	92.82206666	6.0181799185	99	21.38	0.0523	88.54
127184	Tetrachloroethylene (Perchloroethylene)	0.0009927	238	0.00012034	3.4		200	88.85	6.98930782217	85.413618458	7.5970737198	99	48.98	0.0177	166
128665	C.I. Vat Yellow 4	0.024282226	19100	0.00059596	6.28		0.08	98.89	61.9678430579	0	38.032156942	99	6760	8.3e-12	332.36
131113	Dimethyl phthalate	0.0034044	40	0.016503504	1.56		4000	92.18	0.44478194836	0	99.555218052	99	57.5	0	194.19
1319773	Cresol (mixed isomers)	0.33672775	81	0.347071541	1.99		20900	92.37	0.58460539136	0.010826026	99.415394609	99	19.2	0	108.14
132649	Dibenzofuran	0.200647868	8128	0.002578673	4.12		4.22	96.39	18.2902790746	0.2282394439	81.491856002	99	1349	0.00005	168.19
1330207	Xylene (mixed isomers)	0.141174207	1738	0.002578673	3.16		168	96.07	3.02904132403	14.031435412	82.939523264	99	2.17	0.00663	106.17
133062	Captan	0.119134672	198	0.231049	2.35		3.3	76.84	1.52264445601	0.1691827173	98.308172827	99	10	0	300
1335871	Hexachloronaphthalene	0.00116584	32000	0.00011979	7.04		0.0015	99.04	62.3788368336	0	37.611066236	99	346736	0.00009	334.84
1336363	Polychlorinated biphenyls		29495	0.000007	6.4		0.031	98.93	62.0843020317	0.030324472	37.895481654	99.9999	43053	0.000415	371.22
133904	Chloramben		190	0.69	1.9		700	46.32	2.8713298791	0	97.128670121	99	15.49	0	206.03
134292	o-Anisidine hydrochloride		104		1.18			45.63	2.47644093798	0.1314924392	97.392066623	99	4.6	0	159.61
134327	alpha-Naphthylamine	1.305585443	3213	0.005653654	2.25		1698	76.46	1.38634580173	0.013078734	98.600575464	99	30.2	0	143.18
135206	Cupferron	0.272307821	2.7	0.00059596	-1.73		10000000	21.97	6.55439235321	0	93.445607647	99	0.029	0	156.19
137268	Thiram		890	0.005449	1.7		18	75.47	0.98052206175	0.013250298	99.00622764	99	11.5	0	240.41
139139	Nitritotriacetic acid	0.470655493	286	0.002578673	-3.81		59060	92.06	0.35846187269	0	99.630675646	99	1.26	1.2e-16	191
139651	4,4'-Thiodianiline	1.089231284	109	0.011623862	2.18		822	47.11	3.26894502229	0	96.731054978	99	20.42	3.9e-12	216
140885	Ethyl acrylate	0.161501141	22	0.016503504	1.32		15000	92.4	0.40043290043	2.5108225108	97.077922078	99	5.89	0.000393	100
141322	Butyl acrylate	0.165752587	67	0.016503504	2.36		2000	93.02	0.84927972479	2.6230918082	96.516878091	99	8.49	0.00046	128.17

Table 1: Organic Chemicals

CAS Number	Chemical	Air Decay (hr <sup>-1</sup> )	Koc (mL/g)	H2O Decay (hr <sup>-1</sup> )	LOGKow	Kd (L/kg)	Water Solubility (mg/L)	POTW Partition (Removal)	POTW Partition (Sludge)	POTW Partition (Volat)	POTW Partition (Biod)	Incinerator DRE	BCF (L/kg)	Henry's (atm-m <sup>3</sup> /mol)	Molecular Weight
1464535	Diepoxybutane	0.00508308	2.5	0.007001	-0.28		1000000	75.07	0.82589583056	0.026641801	99.160783269	99	0.02	0	86.09
151564	Ethyleneimine (Aziridine)	0.036307709	6	0.000188	-0.28		1000000	45.67	2.36479089118	0.8977446902	96.759360631	99	0.08	0.00001	43
156105	p-Nitrosodiphenylamine	1.524923797	1890	0.005653654	3.16		7.43	58.45	8.65697177074	0	91.343028229	99	269	0	198.22
1582098	Trifluralin	0.058	11070	0.078	5.34		8.11	97.4	58.4496919918	0.030800821	41.509240246	99	3415	0.00003	335
16071866	C.I. Direct Brown 95		187085		7.16			99.68	52.8691813804	0	47.13081862	99		1.0e-24	
1634044	Methyl tert-butyl ether	0.01805051	11.2	0.00059596	0.94		51000	52.94	1.87004155648	24.348318852	73.781639592	99	1.5	0.000587	88
16543558	3-(1-nitroso-2-pyrrolidinyl)pyridine		25		0.32		14.43	45.44	2.39876760563	0	97.623239437	99	0.62	0	177.2
1717006	1,1-Dichloro-1-fluoroethane		464		2.37			90.83	1.06792909832	95.3759771	3.5560938016	99	37	0.0241	116.95
1836755	Nitrofen		4370		4.64		1	96.14	38.2255044726	0	61.774495527	99	1549	0	284.1
1897456	Chlorothalonil		5780	0	3.05		0.6	82.82	3.88794977059	0.036223135	95.12195122	99	501	0	265.9
1937377	C.I. Direct Black 38		11031		4.9			97.89	43.3752170804	0	56.62478292	99	3100	8.2e-40	783.74
2164172	Fluometuron		175	0	2.42		85	48.3	3.89233954451	0	96.128364389	99	28	0	232.21
2234131	Octachloronaphthalene	0.0002371	782000	0.00011979	8.24			99.07	62.4709801151	0	37.529019885	99	44668	0.00019	403.73
2303164	Diallate	0.65729474	273	0.001535743	4.08		14	86.49	24.5230662504	0.046248121	75.430685628	99	140	0	270.24
23950585	Pronamide		984		3.57		15	70.37	14.153758704	0.1563166122	85.689924684	99	300	0	256.14
25321146	Dinitrotoluene (mixed isomers)	0.0766	201	0.13	2.18		270	47.12	3.26825127334	0.042444822	96.689303905	99	27	0	182.15
25321226	Dichlorobenzene (mixed isomers)	0.00309	1700	0.000596	3.47		119.2	75.23	10.46125216	29.482919048	60.055828792	99	260	0.00215	147
25376458	Diaminotoluene (mixed isomers)	1.411966479	61	0.011378973	0.16		35	84.56	0.56764427625	82.887890255	16.544465468	99		0.0113	122.17
2602462	C.I. Direct Blue 6		959		2.95			54.18	6.71834625323	0	93.281653747	99	103	1.0e-24	
26471625	Toluenediisocyanate	1.188	2580	0.693147	3.74			99.48	2.03055890631	0.010052272	97.959388822	99	410	0.00001	174
2832408	C.I. Disperse Yellow 3		3985		3.98		1.18	83.69	22.2009798064	0	77.799020194	99	623	0	269.3
2837890	2-Chloro-1,1,1,2-tetrafluoroethane		245		1.86			99.53	0.42198332161	98.854616698	0.7233999799	99	15.3	0.54	136.48
306832	2,2-Dichloro-1,1,1-trifluoroethane		361		2.17			97.43	0.6568818639	97.998563071	1.3445550652	99	26.3	0.0955	152.93
309002	Aldrin	0.423166777	48500	0.00071205	6.5		0.18	98.96	62.1564268391	0.030315279	37.813257882	99	3890	0.000493	365
3118976	C.I. Solvent Orange 7		28575		6.6		0.0237	99.66	52.6891430865	0	47.310856914	99	11749	0	276.32
334883	Diazomethane		292		2			92.38	0.58454210868	0	99.415457891	99	19.5	0	42.04
34077877	Dichlorotrifluoroethane		361		2.17			97.43	0.6568818639	97.998563071	1.3445550652	99	26.3	0.0955	152.93
353593	Bromochlorodifluoromethane		346	0.18	1.9			97.39	0.48259574905	98.182564945	1.3245713112	99	24.7	0.094	165
354234	1,2-Dichloro-1,1,2-trifluoroethane		361		2.17			97.43	0.6568818639	97.998563071	1.3445550652	99	26.3	0.0955	152.93
354256	1-Chloro-1,1,2,2-tetrafluoroethane		245		1.86			99.53	0.42198332161	98.854616698	0.7233999799	99	15.3	0.54	136.48

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3761533	C.I. Food Red 5		546		2.5			48.85	4.15557830092	0	95.844421699	99	46.8	4.0e-23	482.43
39156417	2,4-Diaminoanisole sulfate		16.2		-0.31			45.43	2.37728373322	0	97.60070438	99		0	234.23
4549400	N-Nitrosomethylvinylamine	0.113098473	20	0.00059596	-0.28		30000	51.08	17.5998433829	19.068128426	78.993735317	99	0.6	0.00041	86.1
463581	Carbonyl sulfide		88		-1.33		1220	96.18	0.30151798711	82.855063423	16.84341859	99	11.2	0.0492	60.07
4680788	C.I. Acid Green 3		64.1		0.79			45.49	2.41811387118	0	97.581886129	99		4.8e-29	690.8
492808	Auramine	1.935182484	2030	0.00059596	2.68		11.02	50.47	4.95343768575	0	95.046562314	99	288	0	267.37
50000	Formaldehyde	0.335021137	37	0.016503504	0.35		400000	92.07	0.36928424025	0	99.619854459	99	1	0	30
505602	Mustard gas	0.020496288	120	9.902103	2.41		684	99.99	0.0300030003	0.010001	99.969997	99	15.5	0.00003	159.08
510156	Chlorobenzilate	0.029325458	1065	0.001375	4.74		13	96.95	40.3713254255	0	59.628674575	99	145	0	325.2
51285	2,4-Dinitrophenol	0.00343339	55.6	0.004591209	1.67		2787	75.45	0.98078197482	0.01325381	99.005964215	99	9	0	184
51752	Nitrogen mustard	0.428349381	91	1.386294	0.91		46700	99.1	0.0706357215	0.010090817	99.919273461	99	4	0	156
51796	Urethane (Ethyl Carbamate)	0.127076983	20	0.0000693	-0.15		480000	45.43	2.37728373322	0	97.60070438	99	0.5	0	89
52686	Trichlorfon	0.350005012	6	0.010315	0.51		154000	92.07	0.36928424025	0	99.63071576	99	0.71	0	257
528290	o-Dinitrobenzene		1.47		1.69		133	45.98	2.67507612005	0	97.303175294	99	0.97	0	168
532274	2-Chloroacetophenone	0.00515874	76	0.002578673	1.93		1572	46.45	2.88482238967	0.2583423036	96.856835307	99	9.77	0	154.59
534521	4,6-Dinitro-o-cresol	0.00122985	238	0.005188602	2.12		198	46.93	3.15363307053	0.1065416578	96.739825272	99	23.99	0	198
53963	2-Acetylaminofluorene	0.52948743	1380	0.00059596	3.12		5.29	57.53	8.25656179385	0	91.760820442	99	171	0	223
540590	1,2-Dichloroethylene	0.014964716	35	0.00059596	2.09		3500	72.25	1.39792387543	64.179930796	34.422145329	99	15.1	0.00408	96.95
541413	Ethyl chloroformate	0.00856699	52.4	1.019542329	0.63			81.95	0.63453325198	30.762660159	68.602806589	99		0.00312	108.53
541731	1,3-Dichlorobenzene	0.00427869	293	0.00059596	3.53		125	77.5	10.4	31.393548387	57.432258065	99	580	0.00263	147
542756	1,3-Dichloropropylene	0.078688	26	0.002556	2.03		2800	82.99	0.9157729847	32.341245933	66.730931438	99	7	0.00355	111
542881	Bis(chloromethyl)ether	1.945055864	17.9	69.31472	0.57		22000	100	0	0	100	99		0.000206	114.97
55185	N-Nitrosodiethylamine	0.129965096	43	0.129965096	0.48		93000	22.14	6.54923215899	0.7678410117	92.682926829	99	1	0	88
55210	Benzamide	0.122977726	13.4	0.008182988	0.64		13500	92.07	0.36928424025	0	99.63071576	99	1.8	0	121
55630	Nitroglycerin	0.216608494	468	0.009283221	1.62		1380	75.4	0.9549071618	0	99.045092838	99	10	0	227
56235	Carbon tetrachloride	0.000024	110	0.00012607	2.83		804.8	92.57	2.11731662526	87.57696878	10.305714594	99	19.95	0.0276	154
56382	Parathion	8.3	10654	0.000722	3.83		6.54	98.36	8.92639284262	0	91.063440423	99	478	0	291.27
569642	C.I. Basic Green 4	10.21717166	97.7	0.00059596	0.8		1000	45.49	2.41811387118	0	97.581886129	99		1.9e-14	364.9
57147	1,1-Dimethyl Hydrazine	0.478226545	4	0.00246146	-1.19		1000000	75.12	0.82534611289	0.2396166134	98.935037274	99	0.043	0	60
57578	beta-Propiolactone	0.00211795	4	0.204468	-0.8		370000	95.91	0.21895527057	0	99.770618288	99	0.45	0	72
57749	Chlordane	0.073352318	38000	0.0000711	6		0.056	98.72	61.5174230146	0.01012966	38.482576985	99	38018	0.00005	409.8
584849	Toluene-2,4-diisocyanate		2580	0.693147	3.74			99.48	2.03055890631	0.010052272	97.959388822	99	410	0.00001	174.15

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58899	Lindane	0.041258761	1081	0.00111034	3.72		7.3	75.38	16.7949058106	0.039798355	83.152029716	99	1259	0	291
593602	Vinyl bromide	0.040556484	170	0.00059596	1.57		4180	94.65	0.22187004754	27.871104068	71.907025885	99	9.18	0.0123	106.95
59892	N-Nitrosomorpholine	0.404335855	1.14	0.205905486	-0.44		861527	45.43	2.37728373322	0	97.60070438	99	0.27	0	116.12
60093	4-Aminoazobenzene	0.393021597	618	0.006069798	3.41		34.6	65.22	11.7295308188	0	88.270469181	99	87	0	197
60117	4-Dimethylaminoazobenzene	1.319138233	7388	0.011695528	4.58		160	95.55	36.8602825746	0	63.139717425	99	1778	0	225
60344	Methyl hydrazine	6.712911884	6	0.001712503	-1.05		1000000	75.08	0.82578582845	0.079914758	99.10761854	99	0.09	0.00003	46
60355	Acetamide	0.119134672	5	0.016503504	-1.26		705000	92.06	0.35846187269	0	99.630675646	99	0.06	0	59
606202	2,6-Dinitrotoluene	0.034249625	100	0.193673477	2.1		182	46.85	3.13767342583	0.064034152	96.81963714	99	12.02	0	182
615054	2,4-Diaminoanisole		20.4		-0.31		19500	45.43	2.37728373322	0	97.60070438	99	0.48	0	138.17
61825	Amitrole	0.119	4.4	0.000596	-0.86		280000	45.42	2.37780713342	0	97.622192867	99		0	84.08
621647	N-Nitrosodi-n-propylamine	2.385241768	28	2.385241768	1.36		9894	45.79	2.51146538546	0.3930989299	97.095435685	99	6.31	0	130
624839	Methyl isocyanate	0.204962876	64.1	4.620981	0.79			99.95	0.020010005	0.140070035	99.83991996	99		0.000926	57.05
62533	Aniline		13.6		0.9		36000	92.09	0.38006298187	0.021717885	99.598219133	99	19.9	0	93.12
62555	Thioacetamide	0.119237168	6	0.016503504	-0.26		163000	45.56	2.37050043898	0.4828797191	97.146619842	99	0.71	0	75
62566	Thiourea	0.238269343	7	0.016503504	-1.08		142000	75.06	0.82600586198	0	99.173994138	99	0.1	0	76.12
62737	Dichlorvos	0.016632	150	0.002666	1.16		10000	75.26	0.86367260165	0.3454690407	98.790858358	99	7.76	0.00001	220.98
62759	N-Nitrosodimethylamine	1.039720771	12	1.039720771	-0.57		1000000	45.46	2.37571491421	0.1319841619	97.492300924	99	0.22	0	74.08
630206	1,1,1,2-Tetrachloroethane	0.00017	92.7	0.0219	2.93		1100	58.8	5.76530612245	68.758503401	25.476190476	99	99.3	0.00242	167.85
63252	Carbaryl	4.667815473	390	0.002063	2.36		82.6	93.29	0.84682173866	5.788401758	93.364776503	99	33.9	0.00131	201.22
636215	o-Toluidine hydrochloride		124		1.32			45.7	2.51641137856	0.1531728665	97.352297593	99	5.93	0	143.61
63938103	Chlorotetrafluoroethane		245		1.86			99.53	0.42198332161	98.854616698	0.7233999799	99	15.3	0.54	136.48
64186	Formic acid	0.00286	12.1	0.0165	-0.54		10000000	92.06	0.35846187269	0	99.630675646	99		0	46.03
64675	Diethyl sulfate	0.105897486	33.5	0.400663	1.14		7000	95.12	0.22077375946	0.052565181	99.72666106	99	4.37	0	154
67561	Methanol	0.0053674	9	0.016503504	-0.77		1000000	92.07	0.35842293907	0.043445205	99.587270555	99	3.02	0	32.04
67630	Isopropyl alcohol	0.060712488	25	0.016503504	0.05		1000000	92.07	0.36928424025	0.086890409	99.554686651	99	0.65	0	60.09
67641	Acetone	0.00136642	18	0.016503504	-0.24		1000000	92.11	0.35826728911	0.3799804581	99.250895668	99	0.39	0.00004	58.08
67663	Chloroform	0.0006119	45	0.00059596	1.97		7950	70.8	1.3418079096	62.231638418	36.426553672	99	8.3	0.00367	119.39
67721	Hexachloroethane	0.00001	2188	0.00059596	3.91		50	77.49	23.0094205704	43.799199897	33.191379533	99	138	0.00389	236.74
680319	Hexamethylphosphoramide		34		0.28		1000000	45.44	2.39876760563	0	97.601232394	99	0.96	0	179
684935	N-Nitroso-N-methylurea	0.722028313	22.5	26.75852797	-0.03		14430	45.43	2.37728373322	0	97.622716267	99	0.56	0	103.09
68768	Triaziquone	0.560633749	20.2	0.007967	-0.13			45.43	2.37728373322	0	97.60070438	99		9.3e-16	231.25
70304	Hexachlorophene	0.0113	288	0.000102	7.54		140	99.06	62.4470018171	0	37.552998183	99		8.6e-13	406.92

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71363	n-Butyl alcohol	0.043335171	72	0.016503504	0.88		63200	92.09	0.38006298187	0.086871539	99.533065479	99	2.75	0	74.12
71432	Benzene	0.0076094	31	0.003790649	2.13		1790	94.09	0.61643107663	18.344138591	81.039430333	99	4.27	0.00555	78.11
71556	1,1,1-Trichloroethane	0.000071	179	0.00015604	2.49		1495	87.75	1.37891737892	93.823361823	4.7977207977	99	8.91	0.0172	133.42
72435	Methoxychlor	0.340384776	80000	0.221713745	5.08		0.04	98.56	46.1038961039	0	53.90625	99	8317	0	345.65
72571	Trypan blue		20.5		-0.12			45.43	2.37728373322	0	97.60070438	99		1.0e-24	960.83
74839	Bromomethane (Methyl Bromide)	0.0002335	106	0.001444	1.19		15220	77.45	0.81342801808	73.699160749	25.487411233	99	4.68	0.00624	94.95
74851	Ethylene	0.06208778	98	0.014956301	1.13		131	99.06	0.28265697557	91.490006057	8.2273369675	99	4.27	0.228	28.05
74873	Chloromethane	0.000259	74	0.002578673	0.91		5325	87.66	0.50193931097	53.593429158	45.916039243	99	2.88	0.00882	50.49
74884	Methyl iodide	0.0007126	158	0.002578673	1.51		13848	75.27	0.94327089146	70.346751694	28.709977415	99	8.32	0.00526	141.95
74931	Methyl mercaptan		21.7		0.78		15390	81.97	0.63437843113	30.779553495	68.573868488	99		0.00313	48.11
74953	Methylene bromide	0.000448	25	0.0000693	1.7		11930	55.71	1.93861066236	30.766469216	67.294920122	99	3.09	0.000861	174
75003	Chloroethane (Ethyl chloride)	0.00238215	37.6	0.00076	1.43		5678	84.39	0.65173598768	82.450527314	16.897736699	99	7.24	0.0111	64
75014	Vinyl chloride	0.03930216	135	0.00059596	1.62		8800	92.41	0.49778162537	90.996645385	8.5055729899	99	10	0.0278	62.5
75058	Acetonitrile	0.0002935	0.28	0.002578673	-0.34		74000	75.27	0.82370134184	0.8237013418	98.352597316	99	0.87	0.00003	41.05
75070	Acetaldehyde		2.19		-0.34		1000000	92.13	0.35818951482	0.6078367524	99.033973733	99	0.4	0.00007	44.05
75092	Dichloromethane	0.0008323	28	0.002578673	1.25		13030	82.2	0.66909975669	31.435523114	67.128953771	99	5.25	0.00325	84.94
75150	Carbon disulfide		65	0	2.14		1185	87.17	0.90627509464	84.730985431	14.374211311	99	11.5	0.0144	76.14
75218	Ethylene oxide	0.0004157	16	0.002407	-0.3		1000000	92.2	0.3579175705	1.1822125813	98.449023861	99	0.35	0.000148	44.05
75252	Bromoform (Tribromomethane)	0.0002935	52	0.00059596	2.4		3100	54.51	3.1370390754	21.060355898	75.802605027	99	3.24	0.000535	252.77
75274	Dichlorobromomethane		51	0	2		6735	64.24	1.68119551681	49.673100872	48.630136986	99	22.9	0.00212	163.8
75343	Ethylidene dichloride		38.3	0.0000693	1.79		5500	76.2	1.01049868766	71.299212598	27.690288714	99	13.5	0.00562	98.96
75354	Vinylidene chloride	0.038518817	343	0.00059596	2.13		2250	92.02	0.74983699196	90.056509454	9.1936535536	99	24.5	0.0261	96.95
75445	Phosgene	0	9.8	7.28	-0.71			100	0	0	100	99		0.00892	98.92
75558	Propyleneimine	0.347762522	11	0.008023	0.13		1000000	75.16	0.82490686535	0.3459286855	98.829164449	99	0.204	0.00001	57
75569	Propylene oxide		25	0.001978	0.03		400000	92.16	0.35807291667	0.87890625	98.763020833	99	0.62	0.000103	58.08
75638	Bromotrifluoromethane (Halon 1301)		245		1.86		320	99.46	0.42228031369	98.833701991	0.7440176956	99	15.3	0.465	149
75650	tert-Butyl Alcohol	0.00646154	37	0.00059596	0.35		1000000	45.74	2.36117184084	1.049409707	96.56755575	99	1.1	0.00001	74.12
75683	1-Chloro-1,1-difluoroethane		81.3		2.05		1397	96.62	0.57959014697	97.847236597	1.562823432	99	21.3	0.0719	100.5
75694	CFC-11 (trichlorofluoromethane)	0	97.7	0.00012	2.53		1000	97.48	1.10791957325	97.466146902	1.4259335248	99	25	0.097	137

Table 1: Organic Chemicals															
CAS Number	Chemical	Air Decay (hr <sup>-1</sup> )	Koc (mL/g)	H2O Decay (hr <sup>-1</sup> )	LOGKow	Kd (L/kg)	Water Solubility (mg/L)	POTW Partition (Removal)	POTW Partition (Sludge)	POTW Partition (Volat)	POTW Partition (Biod)	Incinerator DRE	BCF (L/kg)	Henry's (atm-m <sup>3</sup> /mol)	Molecular Weight
75718	CFC-12 (dichlorodifluoromethane)	0.00018	200	0.000596	2.16		280	99.27	0.59433867231	98.579631309	0.8159564823	99	26	0.343	121
759739	N-Nitroso-N-ethylurea	0.763989878	23.84	26.75852797	0.23			45.44	2.39876760563	0	97.601232394	99	0.88	0	117.1
76017	Pentachloroethane		146.3		3.22		480	57.89	9.84626014856	57.591984799	32.561755053	99	165	0.00194	202.29
76131	Freon 113	0	372	0.00012034	3.16		170	99.53	3.47633879232	95.468702904	1.054958304	99	148	0.526	187.38
76142	CFC 114 (1,2-dichloro,1,1,2,2-tetrafluoroethane)		815	0.17	2.82		130	99.91	1.75157641878	97.507756981	0.7406665999	99	82	2.8	171
76153	CFC 115 (chloropentafluoroethane)		708		2.47		58	99.9	0.93093093093	98.408408408	0.6606606607	99	61	2.66	154
764410	1,4-Dichloro-2-butene		619	0.009025	2.6			90.12	1.48690634709	82.279183311	16.222814026	99	55.7	0.0188	125
76448	Heptachlor	0.387931885	3475	0.006447	5.5		0.18	99.3	50	0.2819738167	49.718026183	99	9550	0.00148	373.35
77474	Hexachlorocyclopentadiene	0.385514443	2000	0.002063	5.04		3.4	98.78	44.826888034	9.8602956064	45.31281636	99	465	0.027	273
77781	Dimethyl sulfate	0.010444684	16	0.577623	0.16		28000	96.97	0.14437454883	0.020624936	99.835000516	99	79.43	0	126
78842	Isobutyraldehyde	0.158846229	8	0.016503504	0.74		89000	92.23	0.36864360837	1.3878347609	98.243521631	99	7.9	0.00018	72
78875	1,2-Dichloropropane	0.00586839	27	0.0000977	2.25		2700	67.88	1.82675309369	55.362404243	42.810842664	99	10	0.00282	113
78886	2,3-Dichloropropene	0.08	77	0.00107	2.42		2750	65.86	2.30792590343	49.559672032	48.147585788	99	1.2	0.00228	111
78922	sec-Butyl alcohol	0.052948743	5.6	0.016503504	0.61		181000	92.08	0.36924413553	0.097741095	99.543874891	99	1.71	0	74.12
78933	Methyl ethyl ketone	0.00593818	5.2	0.016503504	0.29		223000	92.13	0.36904374254	0.5318571584	99.109953327	99	1	0.00006	72
79005	1,1,2-Trichloroethane	0.00194542	79	0.00014578	1.89		4420	39.79	3.59386780598	54.486051772	41.920080422	99	10	0.000824	133
79016	Trichloroethylene	0.014110227	104	0.00012034	2.42		1100	80.97	1.51908114116	90.971964925	7.5089539336	99	17	0.00985	131
79061	Acrylamide		50		-0.67		640000	92.06	0.35846187269	0	99.641538127	99	1	0	71
79107	Acrylic acid	0.153191352	2.19	0.016503504	0.35		1000000	92.07	0.36928424025	0.010861301	99.619854459	99	0.8	0	72
79118	Chloroacetic acid	0.00185966	0.81	0.016503504	0.22		6140000	92.06	0.36932435368	0	99.641538127	99	0.9	0	94
79210	Peracetic acid	0.027625431	7.5	0.088706336	-1.07		712610	92.06	0.35846187269	0.021724962	99.619813165	99	0.12	0	76.05
79221	Methyl chlorocarbonate		28.4	2.038668	0.14			99.63	0.050185687	0.8230452675	99.126769045	99		0.00235	94.5
79345	1,1,2,2-Tetrachloroethane	0.00178974	79	0.03271825	2.39		2962	33.23	6.37977730966	34.84802889	58.80228709	99	8	0.000367	168
79447	Dimethylcarbaryl chloride	0.380551393	9.7	69.31472	-0.72			100	0	0	100	99		0	107.54
79469	2-Nitropropane	0.078281509	20	0.00059596	0.93		17000	75.73	0.83190281262	2.4957084379	96.659183943	99	10	0.000119	110
8001352	Toxaphene	0.0058	6000	0.00019	6.79		0.55	99.01	62.3169376831	0	37.683062317	99	5012	0	431.8
80057	4,4'-Isopropylidenediphenol	0.515176959	1288	0.014530985	3.32		120	85.68	5.99906629318	0	94.000933707	99	10	9.2e-12	228
80159	Cumene hydroperoxide	0.029325458	23	0.002578673	2.16		13900	76.21	1.28592048288	0	98.714079517	99	8.51	0	152
80626	Methyl methacrylate	0.350796136	22	0.002578673	1.38		15000	92.38	0.41134444685	2.2299198961	97.358735657	99	6.6	0.000337	100
81072	Saccharin (manufacturing)	0.381230949	46	0.002578673	0.91		4000	75.13	0.85185678158	0	99.148143218	99	2.88	0	183.18

Table 1: Organic Chemicals															
CAS Number	Chemical	Air Decay (hr <sup>-1</sup> )	Koc (mL/g)	H2O Decay (hr <sup>-1</sup> )	LOGKow	Kd (L/kg)	Water Solubility (mg/L)	POTW Partition (Removal)	POTW Partition (Sludge)	POTW Partition (Volat)	POTW Partition (Biod)	Incinerator DRE	BCF (L/kg)	Henry's (atm-m <sup>3</sup> /mol)	Molecular Weight
812044	1,1-Dichloro-1,2,2-trifluoroethane (HCFC-123b)		361		2.17			97.43	0.6568818639	97.998563071	1.3445550652	99	26.3	0.0955	152.93
81889	C.I. Food Red 15		274		1.95			46.43	2.90760284299	0	97.070859358	99	17.9	1.0e-24	479
82280	1-Amino-2-methyl-anthraquinone	0.173286795	8005	0.006069798	4.07		0.33	86.22	24.2983066574	0	75.701693343	99	1148	1.2e-12	237.25
82688	Quintozene	0.000043	6060	0.0000885	4.64		0.55	89.86	48.3529935455	0.5230358335	51.135099043	99	590	0.00008	295.5
842079	C.I. Solvent Yellow 14	0.116942009	3795	0.002604459	5.51		1.29	99.31	50.1057295338	0	49.894270466	99	1202	0	248.28
84662	Diethyl phthalate	0.018138285	98	0.005071389	2.47		1080	92.95	1.01129639591	0	98.988703604	99	117	0	222
84742	Dibutyl phthalate	0.051517696	160	0.015472035	4.72		13	99.22	29.6109655311	0	70.378955856	99	20.89	0	278
85449	Phthalic anhydride	0.0007861	36	1.540327	1.6		6200	99.3	0.0805639476	0	99.909365559	99	9.68	0	148
86306	N-Nitrosodiphenylamine	0.544615642	1200	0.001868779	3.13		35	57.77	8.34343084646	0.051930068	91.604639086	99	217	0	192
87627	2,6-Xylidine	1.155245301	0	0.005653654	2.17		8240	47.12	3.24702886248	0.1697792869	96.583191851	99	28	0	121
87683	Hexachloro-1,3-butadiene	0.0001331	37153	0.00059596	4.78		3.2	94.82	47.5427125079	18.487660831	33.969626661	99	11400	0.0103	261
87865	Pentachlorophenol	0.00273873	900	0.349724259	5.12		14	96.2	56.2681912682	0	43.731808732	99	766	0	266.5
88062	2,4,6-Trichlorophenol	0.00308939	620	0.176896937	3.69		800	91.33	10.5113325304	0.076645133	89.412022337	99	310	0	197.5
88755	2-Nitrophenol	0.054391831	113	0.002578673	1.79		2185	53.42	2.15275177836	23.961063272	73.886184949	99	13.5	0.000589	160
88891	Picric acid	0.000596	23.6	0.00059596	1.33		13200	22.17	6.85611186288	0	93.143888137	99	1	0	229.11
90040	o-Anisidine	0.719303678	35	0.005634289	1.18		6460	75.19	0.87777630004	0	99.1222237	99	4.6	0	123.16
90437	2-Phenylphenol	3.481489248	119	0.016503504	3.09		700	94.89	2.76109179049	0.010538518	97.217831173	99	15.5	0	170.2
90454185	Dichloro-1,1,2-trifluoroethane		361		2.17			97.43	0.6568818639	97.998563071	1.3445550652	99	26.3	0.0955	152.93
90948	Michlers Ketone	1.906154747	162	0.011623862	3.87		400	60.21	31.7389138017	0	68.277694735	99	20.9	0	268.35
91087	Toluene-2,6-Diisocyanate	1.187635356	2580	0.693147	3.74			99.48	2.03055890631	0.010052272	97.959388822	99	410	0.00001	174.15
91203	Naphthalene	0.12879424	871	0.029603161	3.3		31	95.99	3.93791019898	1.7085113033	94.353578498	99	426	0.000483	128
91225	Quinoline	0.038158102	43	0.006257579	2.03		6110	75.94	1.17197787727	0.065841454	98.762180669	99	7.94	0	129.15
91598	beta-Naphthylamine	1.274753436	203.7	0.005689487	2.28		263	76.56	1.4237199582	0	98.563218391	99	31.6	0	143.18
91941	3,3'-Dichlorobenzidine	18.48392481	190000	18.48392481	3.51		3.11	68.37	13.2075471698	0	86.777826532	99	495	0	253
924163	N-Nitrosodi-n-butylamine	0.872382035	88.4	0.129965096	1.92		1200	46.62	2.85285285285	0.9438009438	96.203346203	99	17	0.00001	158.24
92524	Biphenyl	0.047583181	1500	0.011689982	3.98		7.1	98.86	10.6716568885	0.6170341898	88.711308922	99	436	0.000408	154
92671	4-Aminodiphenyl	0.635384916	185.8	0.016503504	2.86		311	52.74	6.04854000758	0	93.951459992	99	79.4	0	169.22
92875	Benzidine	1.221894068	227000	0.012913199	1.34		360	75.24	0.89048378522	0	99.109516215	99	110	0	184
92933	4-Nitrobiphenyl	0.014067563	2688	0.014956301	3.82		7.36	93.12	12.6181271478	0.010738832	87.371134021	99	436.5	0	199.2
94360	Benzoyl Peroxide	0.00747512	1296	0.016503504	3.46		9.1	96.7	5.18097207859	0.020682523	94.798345398	99	251	0	242
94586	Dihydrosafrole	0.497	2111	0.00258	3.58			70.75	14.3038869258	0.3392226148	85.356890459	99	310	0.00001	164.22

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94597	Safrole	0.635384916	670	0.002578673	3.45		810.67	66.53	12.2801743574	0.3006162633	87.419209379	99	61.6	0	162.18
94757	2,4-D ((2,4-dichlorophenoxy)acetic acid)	0.211794972	109	0.010830425	2.81		890	93.8	1.70575692964	0	98.29424307	99	10	0	221
95476	o-Xylene	0.086643398	129	0.002578673	3.12		178	95.78	2.83984130299	12.00668198	85.163917311	99	21	0.00518	106
95487	o-Cresol	0.238269343	103	0.016503504	1.95		25950	92.35	0.56307525717	0.01082837	99.426096373	99	18	0	108
95501	1,2 Dichlorobenzene	0.00249497	280	0.00059596	3.43		83.96	73.77	10.0040666938	28.371966924	61.637522028	99	270	0.0019	147
95534	o-Toluidine	0.967591242	100	0.019537237	1.32		16600	99.92	0.28022417934	93.975180144	5.7445956765	99	5.9	2.72	107
95636	1,2,4 Trimethylbenzene	0.238269343	2712	0.002578673	3.78		57	94.11	11.4653065562	16.523217511	72.000850069	99	439.5	0.00616	120.19
95807	2,4-Diaminotoluene	1.411966479	36	0.011378973	0.14		300	45.44	2.39876760563	0	97.601232394	99	1.07	0	122
95954	2,4,5-Trichlorophenol	0.01266548	1500	0.69417865	3.72		1200	75.39	16.792678074	0.092850511	83.101207057	99	1905	0	197.5
96093	Styrene oxide	0.030994386	53	0.015753	1.61		3000	75.49	0.95376871109	0.384156842	98.662074447	99	10	0.00002	120
961115	Tetrachlorvinphos		1167	0.00061	3.53		11	88.9	8.29021372328	0	91.709786277	99	283	0	365.95
96128	1,2-Dibromo-3-chloropropane (DBCP)	0.00261133	102	0.00059596	2.96		1230	33.45	13.0343796712	15.216741405	71.77877429	99	11	0.000147	236.5
96333	Methyl acrylate	0.141196648	11	0.016503504	0.8		49400	92.25	0.36856368564	1.4850948509	98.135501355	99	2.4	0.000197	86
96457	Ethylene thiourea	0.766886242	50	0.002578673	-0.66		20000	45.43	2.37728373322	0.022011886	97.60070438	99	10	0	96
97563	C.I. Solvent Yellow 3	0.464915792	347	0.006069798	4.29		100	91.29	29.7294336729	0	70.281520429	99	562.3	0	225.28
98077	Benzotrichloride	0.00219477	492	69.31472	3.9		53	100	0.03	0	99.97	99	98	0.00002	195
98828	Cumene	0.039221291	454	0.009025354	3.66		49.9	98.07	6.93382277965	11.349036403	81.70694402	99	35	0.0115	120
98862	Acetophenone		38.3		1.58		5500	92.2	0.44468546638	0.1084598698	99.436008677	99	9.35	0.00001	120.15
98873	Benzal chloride	0.014119665	209	6.931472	2.97		250	99.99	0.100010001	0.040004	99.859985999	99	27	0.000526	161
98884	Benzoyl chloride	0.00373623	145	17.32868	1.44			100	0.01	0.01	99.98	99	7.32	0.000132	141
989388	C.I. Basic Red 1		38121		5.89			99.54	51.7078561382	0	48.292143862	99	17600	3.0e-14	479.02
98953	Nitrobenzene	0.700792186	229	0.001149618	1.85		1900	92.32	0.51993067591	0.2274696707	99.241767764	99	15	0.00002	123
99558	5-Nitro-o-toluidine	0.193	248	0.015	1.87			46.26	2.831820147	0	97.168179853	99	15.5	0	152.15
99592	5-Nitro-o-anisidine	0.175682465	63.2	0.014956301	1.47		2206	45.76	2.55681818182	0	97.443181818	99	7.67	0	152.71
99650	m-Dinitrobenzene	0.000184	1.39	0.00111	1.49		533	45.78	2.57754477938	0.0218436	97.400611621	99	0.93	0	168

Table 2: Inorganic Chemicals

CAS Number	Chemical	Air Decay (hr <sup>-1</sup> )	Koc (mL/g)	H2O Decay (hr <sup>-1</sup> )	LOGKow	Kd (L/kg)	Water Solubility (mg/L)	POTW Partition (Removal)	POTW Partition (Sludge)	POTW Partition (Volat)	POTW Partition (Biod)	Incinerator DRE	BCF (L/kg)	Henry's (atm-m <sup>3</sup> /mol)	Molecular Weight
7429905	Aluminum (fume or dust)	0	0	0	0	4	0	66.39	100	0	0		79		26.98
7439921	Lead	0	0	0	0	582	0	63.48	100	0	0	91.6	1250		207.19
7439965	Manganese	0	0	0	0	5	0	38.85	100	0	0		0		54.93
7439976	Mercury	0	0	0	0	4084	0	68.57	100	0	0		40000	0.0085	200.59
7440020	Nickel	0	0	0	0	27	0	38.28	100	0	0	99	250		58.71
7440224	Silver	0	0	0	0	539	0	66.47	100	0	0		25		107.87
7440280	Thallium	0	0	0	0		0	53.55	100	0	0		15		204.37
7440360	Antimony	0	0	0	0	9	0	31.51	100	0	0		0.25		121.75
7440382	Arsenic	0	0	0	0	38	0	48.57	100	0	0	97.5	17		74.9
7440393	Barium	0	0	0	0	31	0	69.02	100	0	0		0		137.34
7440417	Beryllium	0	0	0	0	170	0	37.44	100	0	0	97.3	0		9.01
7440439	Cadmium	0	0	0	0	32	0	68.15	100	0	0	88.5	6000		112.4
7440473	Chromium	0	0	0	0	344	0	76.4	100	0	0	99	4000		52
7440484	Cobalt	0	0	0	0	10	0	32.06	100	0	0		4425		58.93
7440508	Copper	0	0	0	0	147	10000	72.47	100	0	0	99.9	14000		63.55
7440622	Vanadium (fume or dust)	0	0	0	0	68	0	31.81	100	0	0		0		50.94
7440666	Zinc (fume or dust)	0	0	0	0	31	0	66.15	100	0	0	99.9	12000		65.38
7664417	Ammonia	0	0	0	-2		899000	59.9					0	0.00002	17.03
7723140	Phosphorus (yellow or white)	0	0	0	0		3.3	59.8	100	0	0		0		30.97
7782492	Selenium	0	0	0	0	22	0	43.66	100	0	0	99.8	2000		78.96
N010	Antimony compounds	0	0	0	0	9	0	31.51	100	0	0		0.25		121.75
N020	Arsenic compounds	0	0	0	0	38	0	48.57	100	0	0	97.5	17		74.9
N040	Barium compounds	0	0	0	0	31	0	69.02	100	0	0		0		137.34
N050	Beryllium compounds	0	0	0	0	170	0	37.44	100	0	0	97.3	0		9.01
N078	Cadmium compounds	0	0	0	0	32	0	68.15	100	0	0	88.5	6000		112.4
N090	Chromium compounds	0	0	0	0	344	0	76.4	100	0	0	99	4000		52
N096	Cobalt compounds	0	0	0	0	10	0	32.06	100	0	0		4425		58.93
N100	Copper compounds	0	0	0	0	147	10000	72.47	100	0	0	99.9	14000		63.55
N420	Lead compounds	0	0	0	0	582	0	63.48	100	0	0	91.6	1250		207.19
N450	Manganese compounds	0	0	0	0	5	0	38.85	100	0	0		0		54.93

Table 2: Inorganic Chemicals

CAS Number	Chemical	Air Decay (hr <sup>-1</sup> )	Koc (mL/g)	H2O Decay (hr <sup>-1</sup> )	LOGKow	Kd (L/kg)	Water Solubility (mg/L)	POTW Partition (Removal)	POTW Partition (Sludge)	POTW Partition (Volat)	POTW Partition (Biod)	Incinerator DRE	BCF (L/kg)	Henry's (atm-m <sup>3</sup> /mol)	Molecular Weight
N458	Mercury compounds	0	0	0	0	4084	0	68.57	100	0	0		40000	0.0085	200.59
N495	Nickel compounds	0	0	0	0	27	0	38.28	100	0	0	99	250		58.71
N725	Selenium compounds	0	0	0	0	22	0	100	0	0	0	99.8	2000		78.96
N740	Silver compounds	0	0	0	0	539	0	66.47	100	0	0		25		107.87
N760	Thallium compounds	0	0	0	0		0	53.55	100	0	0		15		204.37
N982	Zinc compounds	0	0	0	0	31	0	66.15	100	0	0	99.9	12000		65.38

Table 3: Chemicals Missing POTW Removal Efficiencies

CAS Number	Chemical	Air Decay (hr <sup>-1</sup> )	Koc (mL/g)	H2O Decay (hr <sup>-1</sup> )	LOGKow	Kd (L/kg)	Water Solubility (mg/L)	POTW Partition (Removal)	POTW Partition (Sludge)	POTW Partition (Volat)	POTW Partition (Biod)	Incinerator DRE	BCF (L/kg)	Henry's (atm-m <sup>3</sup> /mol)	Molecular Weight
74908	Hydrogen cyanide	0.00017823	17.4	0.00059596	-0.25		1000000	71.98	1.64	1.84	96.63	0	0.38	0.000133	27
85687	Butyl benzyl phthalate	0.063538492	17000	0.016503504	4.91		2.69	96.76	43.42	0.1	56.48	99	663	0	312
12427382	Maneb		550		0.62		6	71.98	1.64	1.84	96.63	99		0	265.3

Table 4: Chemicals Missing Some Physicochemical and Removal Efficiencies Data

CAS Number	Chemical	Air Decay (hr <sup>-1</sup> )	Koc (mL/g)	H2O Decay (hr <sup>-1</sup> )	LOGKow	Kd (L/kg)	Water Solubility (mg/L)	POTW Partition (Removal)	POTW Partition (Sludge)	POTW Partition (Volat)	POTW Partition (Biod)	Incinerator DRE	BCF (L/kg)	Henry's (atm-m <sup>3</sup> /mol)	Molecular Weight
N084	Chlorophenols		73		2.18		28500	72.87	6.53	1.86	91.6	99		0.00001	128.56
N106	Cyanide compounds						10000000							0.000122	

Table 5: Chemicals Missing Significant Amounts of Data

CAS Number	Chemical	Air Decay (hr <sup>-1</sup> )	Koc (mL/g)	H2O Decay (hr <sup>-1</sup> )	LOGKow	Kd (L/kg)	Water Solubility (mg/L)	POTW Partition (Removal)	POTW Partition (Sludge)	POTW Partition (Volat)	POTW Partition (Biod)	Incinerator DRE	BCF (L/kg)	Henry's (atm-m <sup>3</sup> /mol)	Molecular Weight
10034932	Hydrazine sulfate						34150								130.13
10049044	Chlorine dioxide														67.45
123677	Paraldehyde						125000					99			132.16
1313275	Molybdenum trioxide						490								143.95
1314201	Thorium dioxide						0								264.05
1332214	Asbestos (friable)														554.22
1344281	Aluminum oxide (fibrous forms)						0.98								102
156627	Calcium cyanamide	0.119134672	8.53	0.002578673	-0.82		0								80.11
20816120	Osmium tetroxide						57000								254.1
302012	Hydrazine	0.57642561	4.28	0.016503504	-1.37		1000000						0.02		32
6484522	Ammonium nitrate (solution)						1183000								80.04
74456	Chlorodifluoromethane (HCFC-22)											99			86.47
7550450	Titanium tetrachloride														189.73
7647010	Hydrochloric acid														36.46
7664382	Phosphoric acid	0.38													98
7664393	Hydrogen fluoride				-0.44		10000000								20.01
7664939	Sulfuric acid						10000000								98.08
7697372	Nitric acid						10000000								63.01
7782505	Chlorine						9460								70.9
7783064	Hydrogen sulfide						4132								34.08
8001589	Creosote, coal tar						0					99			
81812	Warfarin and salts														308.32
N230	Glycol Ethers														
N575	Polybrominated Biphenyls (PBBs)	0.06	37535	0.06	7.8		0.02	92	24	10	66	99	18200		628
None1	Ethylenebisdithiocarbamic acid, salts and esters														

## **Appendix E.**

### **Considerations for Including Underground Injection in the TRI Risk-Related Chronic Human Health Indicator**

## Considerations for Including Underground Injection in the TRI Risk-Related Chronic Human Health Indicator

### 1. Background Information on Underground Injection

Underground injection refers to the placement of fluids into permeable rock strata in the subsurface environment using wells. Disposal of industrial wastes through the use of underground injection began in the 1930's. This practice is based on simple hydrogeological principles and has been considered a useful method of isolating wastes from the accessible environment by placing them into deep formations where they will remain for millions of years.

EPA classifies five types of underground injection wells. These are:

Classification	Definition <sup>3</sup>	1992 Inventory <sup>4</sup>
Class I	wells that inject municipal or industrial waste water (including hazardous waste) below the lowermost underground sources of drinking water (USDW) <sup>5</sup>	517 active wells (170 hazardous)
Class II	wells that inject fluids related to oil and gas production, including saltwater disposal, enhanced oil recovery and liquid hydrocarbon storage	177,047 active wells
Class III	wells that inject fluids for the extraction of minerals	35,668 active wells
Class IV	wells that inject hazardous waste into or above a USDW (these wells have been banned)	409 abandoned wells

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<sup>3</sup>Definitions taken from *U.S. EPA Fact Sheet: Underground Injection Control*, Office of Drinking Water.

<sup>4</sup>Underground Injection Control Program, *Injection Well Inventory, 1992*, Office of Groundwater and Drinking Water.

<sup>5</sup>A USDW is defined as an aquifer that is currently serving as a public drinking water supply, or those that have the potential to serve as a public drinking water supply, and have less than 10,000 mg/L total dissolved solids.

Classification	Definition <sup>6</sup>	1992 Inventory <sup>7</sup>
Class V	wells that do not fit into any of the above categories, including industrial dry wells and aquifer remediation wells	190,443 active wells

The Underground Injection Control (UIC) program was established in 1974 to protect USDWs from contamination due to underground injection practices and is administered under the Safe Drinking Water Act (SDWA). Many types of underground injection, however, are also defined as a form of hazardous waste land disposal and thus are subject to the land disposal restrictions imposed by the Hazardous and Solid Waste Amendments of 1984 (HSWA). The HSWA banned all injections into Class I Hazardous Waste (Class 1H) wells. However, EPA may allow injections to continue if it determines that the prohibition is not required to protect human health and the environment.

Pursuant to HSWA requirements, in 1985 EPA conducted an inventory of Class I facilities and summarized their results in the *Report to Congress on Underground Injection*<sup>8</sup>. In 1986, EPA evaluated reported failures and incidents of noncompliance using data gathered in Report to Congress and studies conducted by Engineering Enterprises<sup>9</sup>, and the Underground Injection Practices Council (UIPC), an independent coalition of industry, government, and consulting professionals. From these reports, EPA concluded that "most USDWs are adequately separated from injection zones and that contamination of USDWs from injection operations is insignificant."<sup>10</sup> When contamination incidents did occur, the problems were the result of improper well design and construction, or poor operation standards and/or monitoring requirements. EPA believes that these failures would not have occurred under better management standards. To further protect USDW from potential underground injection failures, in July of 1988 EPA promulgated more stringent technical requirements for Class 1H wells. These regulations are published in 40 CFR parts 124, 144, 145, 146, and 148, and are summarized below.

Most of the 1988 regulations stipulate safe practices for operating Class 1H wells that will prevent contamination of USDWs. Before a Class 1H well can begin operations, however, the operator must prove to EPA that the injection operations will not endanger human health and the environment by submitting a "no-

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<sup>6</sup>Definitions taken from *U.S. EPA Fact Sheet: Underground Injection Control*, Office of Drinking Water.

<sup>7</sup>Underground Injection Control Program, *Injection Well Inventory, 1992*, Office of Groundwater and Drinking Water.

<sup>8</sup>U.S. EPA 1985. *Report to Congress on Injection of Hazardous Waste*. Office of Drinking Water. EPA 570/9-85-003.

<sup>9</sup>*Class I Hazardous Waste Well Failure Study Prepared for U.S. Environmental Protection Agency*. Prepared by Engineering Enterprises, Inc., Geraghty & Miller, Inc., and Ken E. Davis Associates, September, 1986.

<sup>10</sup>U.S. EPA, Office of Drinking Water (1986). Class I Hazardous Waste Injection Wells Evaluation of Non-compliance Incidents.

migration" petition demonstrating that the waste will not migrate from the injection zone for as long as it remains hazardous. Well operators that do not submit petitions must either treat to remove the banned substances or cease injection of the waste. The "no-migration" petitions are comprehensive, typically several volumes long and containing thousands of pages of technical data. Petitions are required to address every technical aspect of well siting, construction, operation, and a detailed analysis of the injected waste streams. EPA has established a rigorous Class 1H petition review process; approximately 2000 hours are spent on each petition review. Prior to the approval of any petition, EPA reviews the construction, operation, compliance history, and closure plans for the well. In addition, they evaluate the chemical compatibility of the waste with the materials of the well construction, and the injection and confining zone rocks and fluids. Information for the Area of Review (AOR) is studied to ensure that no migration could occur through unplugged or improperly completed wells which penetrate the confining zone.

The Class 1H operating requirements were designed to control underground injection contamination pathways. The following summary of the technical requirements has been taken directly from the EPA's Office of Ground Water and Drinking Water publication, *Analysis of the Effects of EPA Restriction on the Deep Injection of Hazardous Waste*<sup>11</sup>.

The controls to prevent well failure include:

- The well materials must be compatible with wastes they are likely to contact and operators are required to conduct corrosion monitoring.
- The wells must be adequately cased and cemented to protect USDWs and isolate the injection zone.
- The long string casing, injection tubing, and annular seal must be pressure-tested at least annually, and whenever there is a well workover. The bottom-hole cement must be tested annually by a radioactive tracer survey (RTS). Also, a test for fluid movement along the bore hole must be conducted at least once every five years using a noise, temperature, or other EPA-approved logging method. Finally, for certain Class I wells, casing inspection logs must be maintained. These logs are predictive tools to assess developing weaknesses in the well's casing.
- The operator must install and use continuous recording devices to monitor the waste injection pressure, flow rate and pressure. He must also install and use an automatic alarm and shut-down system designed to alert the operator and shut-in the well when pressures, flow rates, or other parameters exceed the allowable limits.
- If loss of mechanical integrity is found during an automatic shutdown or during routine MIT, the operator must notify the EPA, cease injecting fluids, and preform the well workover and remediation plan specified by the director.

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<sup>11</sup>U.S. EPA 1991. *Analysis of the Effects of EPA Restrictions on the Deep Injection of Hazardous Waste*. Office of Ground Water and Drinking Water. EPA 570/9-91-031.

Controls to prevent fluid migration up improperly plugged wells that penetrate the confining zone include:

- The operator must identify all wells within a two-mile radius of the well bore. In some cases a larger area of review (AOR) may be required if pressure analysis shows that the injection well has a greater radius of influence.
- All wells on the AOR must be examined to determine whether they are adequately completed or plugged, or that there is no potential for fluid movement.
- A description of each well and any records of its plugging or completion must be submitted to EPA. A remediation plan must be submitted for wells that EPA determines are improperly plugged, completed, or abandoned, or for which plugging or completion information is inadequate. The plan must consist of steps or modifications that will be taken to ensure that fluids will not move up the wells. The plan is be a condition of the operating permit.

Controls to prevent fluid migration through faults or fractured confining strata include:

- Wells must be completed such that the injection zone which receives the waste is confined above and below by an impermeable confining zone.
- Injection pressure must be controlled so that new fractures are not created or propagated in the injection zone or the confining strata.
- The confining zone must be laterally continuous and free of faults and transmissive fractures.
- The waste must be chemically compatible with the confining zone, so that dissolution of the confining zone rock does not allow waste to migrate out of the injection zone.
- The operator must conduct an annual pressure transient test to measure any changes in reservoir characteristics and the pressure increase in the reservoir over time.

Controls to prevent lateral displacement of fluids include:

- The injection zone must have sufficient permeability, porosity, thickness, and areal extent to prevent fluid movement into USDWs.
- Information must be provided by the operator on faults, the continuity of injection and confining zones, and the proximity of USDWs to the injection well.

## **2. Human Health Risk Analysis**

The fundamental problem with analyzing the human health risks from current underground injection practices is that well-maintained and well-operated facilities in theory pose little or no human health risks since the

potential for exposure is removed. In fact, a letter from the UIPC urged EPA not to consider injection into deep wells as a "release" to the environment for this reason<sup>12</sup>. In fact, there are only a few documented cases of well failures where underground sources of drinking water have been contaminated. For example, EPA and state regulatory agencies have identified two cases where injected wastes contaminated USDWs, and one case where an injection well was suspected of causing contamination of an USDW. All three cases occurred prior to the implementation of a State or Federal UIC program. EPA has also identified eight cases where leakage from Class 1H wells entered non-USDW formations and two cases of surface contamination due to blowouts.

Both cases of known USDW contamination from Class 1H injection wells occurred prior to the existence of the UIC program. Both wells failed due to the same problem; they were constructed without a tubing and packer and without a surface casing set to protect the area's USDWs. Corrosion of the long string casing (the only layer of protection for these wells) allowed the unobserved leakage of wastes into USDWs. The UIC regulations currently in effect would never have allowed this method of completion for Class 1H wells. As was stated above, UIC regulations require three redundant layers of protection: a surface casing set and cemented through all USDWs, a cemented long-string casing, and a tubing with a packer (or an equivalent). These three levels of protection and the requirement for continuous annulus pressure (mechanical integrity) monitoring would make these cases of contamination impossible today.

In another incident, Class 1H injection wells operated by Hammermill Paper were suspected as the cause of USDW contamination near Erie, PA in 1972. It was suspected, but never proven, that the increase in injection zone pressure attributable to the Hammermill wells caused injected waste or formation fluid to migrate up an unplugged well into an USDW, five miles from the injection site. The current UIC regulations require that the pressure effects of an injection well be thoroughly examined. Also, in an area where injection pressures are found to be sufficient to cause migration to an USDW, the operator is required to identify and evaluate all artificial penetrations of the confining zone. Furthermore, the Land Disposal Restrictions regulations require a detailed analysis of the fate and transport of the injected waste, and an evaluation of its potential for confinement in the injection zone for 10,000 years. Given the relatively shallow injection zone of the Hammermill wells, it is highly unlikely that the petitions for these wells would have been approved under the current UIC program.

Hazardous waste leakage out of the injection zone into non-USDWs also occurred in the past. Eight facilities between 1975 and 1984 reported such incidents. Most of these failures occurred prior to the implementation of UIC programs and were relatively minor leaks in the area immediately adjacent to the well bore. All incidents were caused by tubing and casing corrosion. The most notable of these cases involved the unobserved deterioration of the long-string casing in wells without packers at the Chemical Waste Management site in Vickery, Ohio in 1983. This type of failure is easily detected with continuous annulus pressure monitoring. However, the Chem Waste wells were designed in such a manner that it was not possible to conduct this type of continuous monitoring. Current UIC regulations require either a packer or a system that allows comparable protection and a capability for continuous monitoring of mechanical integrity. In all eight cases where leakage into non-permitted zones occurred, the current UIC program's construction, monitoring, and MIT requirements would have either prevented the failure or detected its occurrence in time to prevent significant leakage.

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<sup>12</sup>Letter from L. Wilcher to R. Thomas Segall, President of Underground Injection Practices Council, September 30, 1991.

In addition, there have been two cases of well blowouts which resulted in soil contamination at the surface. Both of these cases were caused by the buildup of CO<sub>2</sub> gas that was generated in the injection zone due to the incompatibility of the injected waste with the formation. The two blowouts occurred before the implementation of a UIC program in the states where the incidents occurred. As was stated previously, current UIC regulations require that an operator demonstrate the compatibility of the waste with the materials of well construction and with the injection formation. The regulations also require the operator to demonstrate the capability for emergency shut-in in case of well failure or in response to conditions such as those encountered in these two examples.

An analysis of potential health risks from the failure of a Class 1H injection well would have to involve a calculation of both the probability of a failure event occurring and the level of exposure should the failure occur. As has been illustrated from an explanation of past well failures, the probability for such events to occur while the Class 1H injection facilities are under the management of an UIC program are extremely small. In fact, the UIC program controls are so protective, that if the program is operating properly, these risks are most certainly negligible. However, because some TRI wastes are not regulated under RCRA as hazardous wastes, some TRI facilities that release waste fluids through underground injection are not Class 1H. In addition, some TRI facilities may be operating underground injection wells that are classified as Class V. Thus, these "RCRA-non-Haz Waste" TRI facilities as well as any TRI Class V wells are not subject to the stringent UIC requirements outlined above and may pose some risk of human exposure due to failure.

### **3. Evaluating Underground Injection in Indicator**

The current Indicators model tracks only pounds of releases to underground injection. Project staff is currently investigating other possibilities for including these releases in the Indicator. One possibility is to include the releases only in the version of the computer algorithm that multiplies the pounds released times the toxicity weighting factor for the chemical. This would track changes in underground injection practices over time. However, the interpretation of such an Indicator would have to be considered carefully. If in fact underground injection represents a more safe way of handling toxic chemicals than other releases, then an increase in a pounds-times-toxicity weight Indicator may actually represent a decrease in overall health and environmental impacts, if toxic chemicals were being moved to underground injection from media with higher potential for impacts.

Another possibility would be to try to include exposure potential for underground injection in the Indicator. Beginning with the 1996 reporting year, facilities must report whether releases to underground injection are placed in Class I facilities or in Class II-V facilities. Some modeling has been performed for Class I underground injection failures for different geographical settings and for different failure scenarios where a ratio between the injected concentration and the concentration in the drinking water aquifer were obtained. These ratios could be applied to the TRI releases to Class I facilities to estimate aquifer concentrations, and subsequently surrogate doses through drinking water. The probability of failure could be estimated from the failure rates reported in the UIPC report and a consideration of current practices. However, exposure potential for other types of facilities would remain unknown.

Project staff will obtain additional updated information regarding underground injection. With new information, additional alternatives will be developed and evaluated for including underground injection in the Indicator.

## **Appendix F**

### **Waste Volumes by Industry**

### Number of Landfills by Amount of Waste Received in 1984

Waste Type	Survey Response Rate	Quantity of Waste Received			Total Landfills Per Waste Type*
		<30,000 cu yds (<30,000 tons/day)	30,000-600,000 cu yds (30-50 tons/day)	>600,000 cu yds (>500 tons/day)	
Municipal Solid Waste	85%	5,309 (67%)	2,211 (28%)	408 (5%)	7,925 (100%)
Industrial Waste	82%	2,289 (79%)	523 (18%)	72 (2.5%)	2,884 (100%)
Demolition Waste	83%	1,608 (75%)	468 (22%)	78 (3.6%)	2,154 (100%)
Other Waste	85%	790 (93%)	51 (6%)	11 (1.3%)	852 (100%)

Source: U.S. EPA. 1988. Report to Congress: Solid Waste Disposal in the United States, Volume 1, Draft Final (Revised), April 15, 1988.

\* = Percentages may not total 100 percent due to rounding.

Number of Industrial Establishments with Landfills by Annual Waste Quantity Disposed in Them in 1985

Industry Type	Number of Establishments by Annual Quantity of Waste Disposed of in Landfills in 1985 (thousand tons)						
	Less than 0.5	0.5-5	5.1-20	21-100	101- 1,000	More than 1,000	Total Establishments Per Industry Type <sup>a</sup>
Organic Chemicals	2	4	4	2	1	0	13
Primary Iron and Steel	69	55	29	13	9	0	176
Fertilizer & Agricultural Chemicals	25	2	0	0	2	1	30
Electrical Power Generation	23	13	6	23	57	3	126
Plastics and Resins Manufacturing	18	6	2	2	0	0	28
Inorganic Chemicals	30	31	10	9	0	1	81
Stone, Clay, Glass, & Concrete	873	129	85	46	10	0	1,143
Pulp & Paper	26	14	83	44	12	0	179
Primary Non-ferrous Metals	32	35	7	13	2	0	90
Food and Kindred Products	127	22	17	12	11	0	189
Water Treatment	33	33	0	3	0	0	69
Petroleum Refining	21	9	8	1	1	0	40
Rubber and Misc. Products	2	22	2	10	0	0	36
Transportation Equipment	37	8	7	7	1	0	54
Selected Chem. and Allied Products	6	6	6	1	0	0	19
Textile Manufacturing	12	6	7	0	0	39	25
Leather and Leather Products	8	0	1	0	0	0	9
Total <sup>a</sup>	1,344	396	274	181	105	5	2,305 <sup>b</sup>

Source: U.S. EPA. 1988. Report to Congress: Solid Waste Disposal in the United States, Volume 1, Draft Final (Revised), April 15, 1988.

<sup>a</sup> = These are the correct totals. Table entries may not add to their respective totals due to rounding.

<sup>b</sup> = Overall response rate for this table is 99.3%.

Number of Industrial Establishments with Surface Impoundments by  
Industry and Waste Quantity Disposed in Them in 1985

Industry Type	Number of Establishments by Waste Quantity Disposed of in Them in 1985 (tons)								
	Less than 3	3-9	10-99	100- 499	500- 999	1,000- 4,999	5,000- 10,000	Greater than 10,000	Total Establish- ments Per Industry Type <sup>a</sup>
Organic Chemicals	1	2	2	12	1	11	13	45	86
Primary Iron and Steel	1	1	37	18	3	24	10	89	182
Fertilizer & Agricultural Chemicals	3	1	37	9	3	6	3	47	110
Electrical Power Generation	5	3	29	29	7	20	7	207	306
Plastics and Resins Manufacturing	3	2	4	6	1	8	2	50	77
Inorganic Chemicals	3	1	25	34	14	83	32	145	340
Stone, Clay, Glass, & Concrete	42	106	419	594	194	217	76	290	1,939
Pulp & Paper	9	23	0	29	3	19	15	201	301
Primary Non-ferrous Metals	6	5	38	18	2	51	10	55	186
Food and Kindred Products	13	30	105	215	54	353	129	799	1,700
Water Treatment	0	0	34	34	5	17	32	207	329
Petroleum Refining	30	4	60	12	10	70	8	117	310
Rubber and Misc. Products	41	1	22	1	10	1	3	46	126
Transportation Equipment	7	0	19	29	2	9	8	44	118
Selected Chem. and Allied Products	2	0	2	3	4	4	5	33	52
Textile Manufacturing	1	16	39	1	11	21	16	283	388
Leather and Leather Products	0	0	3	3	1	0	1	18	27
Total <sup>a</sup>	168	197	877	1,049	325	916	369	2,677	6,578 <sup>b</sup>

Source: U.S. EPA. 1988. Report to Congress: Solid Waste Disposal in the United States, Volume 1, Draft Final (Revised), April 15, 1988.

<sup>a</sup> = These are the correct totals. Table entries may not add to their respective totals due to rounding.

<sup>b</sup> = Overall response rate for this table is 98.5%.

Number of Establishments with Waste Piles by Industry Type  
and Waste Quantity Disposed of in Them in 1985

Industry Type	Number of Establishments According to Amount of Waste Disposed in Them (thousand tons)						
	Less than 0.5	0.5-5	5.1-20	21-100	101-1,000	More than 1,000	Total Establishments Per Industry Type <sup>a</sup>
Organic Chemicals	21	15	2	0	0	0	37
Primary Iron and Steel	202	74	24	14	2	2	317
Fertilizer & Agricultural Chemicals	19	2	4	1	3	1	30
Electrical Power Generation	77	8	0	8	1	0	93
Plastics and Resins Manufacturing	19	1	2	0	0	1	23
Inorganic Chemicals	30	12	4	2	7	4	60
Stone, Clay, Glass, & Concrete	1,549	184	131	57	21	0	1,942
Pulp & Paper	51	63	38	7	2	0	162
Primary Non-ferrous Metals	198	41	14	4	3	1	261
Food and Kindred Products	297	28	4	11	0	0	340
Water Treatment	41	1	0	0	0	0	42
Petroleum Refining	112	21	2	0	0	0	135
Rubber and Misc. Products	76	21	1	0	0	0	98
Transportation Equipment	213	70	15	2	1	0	300
Selected Chem. and Allied Products	33	6	0	0	0	0	39
Textile Manufacturing	90	10	0	0	0	0	99
Leather and Leather Products	37	3	0	0	0	0	39
Total <sup>a</sup>	3,064	558	242	106	40	9	4,019 <sup>b</sup>

Source: U.S. EPA. 1988. Report to Congress: Solid Waste Disposal in the United States, Volume 1, Draft Final (Revised), April 15, 1988.

<sup>a</sup> = These are the correct totals. Table entries may not add to their respective totals due to rounding.

<sup>b</sup> = Overall response rate for this table is 99.3%.

## **Appendix G**

### **Options for Indicator Computation and Normalization**

## I. Options for Indicator Computation

The TRI indicator will be calculated by combining the individual scores of the TRI chemical-facility-media components. Each component's value is related to a chemical's risk to either human health or the environment (depending on the indicator). The value is calculated based on measures of the volume of release from a facility, the chemical's toxicity, and the potential exposed population for the media of release.

This appendix discusses the two leading methodologies considered for calculating the TRI indicator. The method of calculation will influence the ways we can adjust the indicator and how the indicator will change in response to the adjustments as facilities and chemicals are added over time.

### Simple Sum of the Component Scores:

$$I = S_1 + S_2 + S_3 + \dots + S_n$$

where:

$I$  = TRI indicator  
 $S$  = facility-chemical-medium-specific subindicator

In this method, each component score makes a contribution proportional to its size. Simply, it is the total "risk" resulting from all chemical-facility-media releases. It should be noted that subscores for particular chemicals, industries, and regions can also be calculated for indicator diagnostics.

### Simple Sum Normalized to a Base Year:

$$I = \frac{(S_1 + S_2 + S_3 + \dots + S_n)_{\text{present year}}}{(S_1 + S_2 + S_3 + \dots + S_n)_{\text{base year}}} \cdot 100\%$$

Like the simple sum method, this method represents each component score proportionately. Its primary advantage is that it is a dimensionless ratio that tracks progress over time and continuously looks back at the beginning of the indicator record. A score of 60 indicates that the overall chemical-facility-media risk has been reduced by 40 percent since the TRI indicator began. Hence, each individual score has meaning, as does the change from year to year.

## **Other Methods of Calculation**

We considered alternative means of calculating the indicator. Some of these included the arithmetic mean of the component scores, the geometric mean of the scores, and the least-square difference of the scores. Although each of these methods generates a score that will fluctuate as the individual components of the risk, the methods do not produce readily interpretable results.

For the greatest sensitivity in the actual indicator score, as well as for the greatest ease in calculation and interpretation, we recommend that the chemical-facility-media scores simply be added and then adjusted to a manageable level.

## **II. Normalizing the Indicator**

This section discusses options considered for modifying the indicator to accommodate the addition of SIC codes and chemicals for TRI reporting purposes. We discuss how the failure to report chemical release data as well as data errors can affect the calculation of the indicator. We also present an example to illustrate both the necessity of designing a method of normalization and the implications of the methods presented here.

As discussed previously, the indicator should be designed to accommodate an increase in the number of components of the TRI. This increase can occur through any of three mechanisms: an addition of chemicals to the TRI list, an increase in the number of facilities by enhancing the SIC code list, and an increase in facility compliance with existing reporting requirements. Each of these scenarios enhances the accuracy of the report because they supply missing information. However, this addition changes the scope of the indicator (from a small subset to a larger subset), thereby limiting the effectiveness of comparison between current and past values.

The addition to or deletion of chemicals from the TRI roster will occur as EPA responds to petitions or initiates its own action through the chemical listing or delisting process. The deletion of chemicals will presumably have a minor effect since such chemicals would be deleted due to their low risk; by definition these chemicals will make only a minimal contribution to the indicator. Deletion will most likely occur in batches every few years. The addition of SIC codes will likely follow investigations of the TRI chemicals revealing other industries that emit the listed chemicals. Compliance could also increase in the future. In 1989, the Office of Toxic Substances studied compliance with TRI reporting requirements. The study found that the compliance rate was 81.7 percent in the first year of reporting. Follow up studies have not been done to determine the improvement in compliance with Section 313. However, the OTS study stated that under full compliance, the estimated number of respondents would be over 29,000. In the last two years of reporting, the number of reporting facilities has not approached that figure, despite a lowering of reporting thresholds.

The fundamental problem in maintaining a single, continuous indicator is that there is no way to differentiate between fluctuations due to changes in actual environmental risk and those due to changes in the chemical or facility roster. Therefore, to maintain the integrity of the indicator when chemicals are added to the roster, each addition to the indicator should be accompanied by some kind of adjustment. Methodologies

for accommodating the addition of chemical-facility-media components are presented below along with discussions of their impact on the accuracy of the indicator. First, we present a hypothetical example of indicator values over a five year period and then articulate a number of options for normalizing the index.

Example:

The calculation of the indicator begins in 1988, and we select the Simple Sum method of calculating the indicator. For the first 5 years the indicator scores are as follows:

Year	Indicator Score
1988	1,000
1989	950
1990	850
1991	800
1992	775

In 1993, the Agency adds another 200 chemicals to the TRI list as well as five SIC codes. The 1993 score of the original set of TRI chemicals and SIC codes is 750, meaning that the risks associated with those chemicals and facilities have decreased. The score for the additional set of chemicals and facilities is 500.

**Do Nothing**

The Do-Nothing scenario is important to examine since the benefits of lost continuity may outweigh the disadvantages and the effort required to work around them. For this method, the score will rise when components are added and will no longer describe the environmental progress as compared to the previous roster. In our example, the indicator score will read 775 in 1992 and 1,250 in 1993. It will be impossible to recalculate the previous years' scores with the new chemicals because release data will not be available. Thus, information on progress since the initial roster will be lost.

The Do-Nothing scenario could be viewed as a more accurate representation of the "complete picture" of environmental risk. If, for example, the indicator score for the universe of **all** chemicals and **all** facilities were actually 4,000, and this initial TRI setup provides a score of 1,000, then the subsequent addition of components to the TRI will fill in the additional 3,000 points for which no information exists. Yet for the public to understand the severity of a change, increases in the indicator score from new chemicals ought to occur on the same scale as that of the original set. As discussed earlier, the public will perceive the indicator score presented with the first set of TRI chemicals and facilities as representing the risk associated with all chemicals and facilities. The public will believe that the new score of 1250 means that the risks posed to them have risen by 475 points; actually, the risk to them has not increased at all, they are just better represented. An increase in the number of components should not actually increase risk but should redistribute the individual contributions to the total risk.

### **Creation of a Separate Indicator**

Chemicals could be added to the TRI roster one or two at a time each year or in a large number once every five years. If the latter occurs exclusively, we could establish an indicator consisting solely of the new chemicals and allow the scores of the old indicator to continue as before. In our example, the TRI indicator would be reported as two scores: in 1993 it would be 750 for the original set of TRI chemicals and facilities and 500 for the new set of chemicals and facilities. This approach has two advantages. First, this system could accurately track the progress of the original roster as well as the new roster. Second, the indicator for each roster could be compared and the program could establish priority for alleviating environmental problems associated with the new or old list.

The primary disadvantage of two indicators is the loss of a single instrument. Chemicals and SIC codes will be added to the TRI more than once, and each time another four indices (human health and environmental risk; chronic and acute effects) will be needed. Each of these indices is also compared at regional, state and local levels. Maintaining a number of indicators will create public confusion, as people try to keep track of each separate indicator change from the previous year. A second disadvantage follows from the Do-Nothing scenario: if people add these scores together to get the "total" score, they will perceive an increase in overall risk. Finally, if TRI chemicals are added continuously in small amounts, this method will be extraordinarily difficult to implement as new indices are created each year.

### **Ratio Adjustment**

The ratio adjustment method is used with the Dow Jones Industrial Average, the Producer Price Index, the Consumer Price Index, and the New York Stock Exchange Composite Index. The underlying components of each of these indices are updated periodically to reflect fundamental shifts in what is being measured. For example, this year the Dow substituted three service sector stocks for three industrial stocks to reflect the U.S. economy's shift toward the service sector. The Producer and Consumer Price indices revise their basket of goods decennially to reflect the caprice of consumer taste. The NYSE Composite Index, which encompasses every stock on the New York Stock Exchange, is revised every time companies start up, merge, or fail.

The adjustment is straightforward. On the first day that the revised components are employed, the index is calculated twice, once based on the old components and again based on the revised components. Thereafter, the ratio between these two index values is used to adjust the index as it is calculated from the revised components:

$$I = I_{\text{revised components}} \cdot \frac{I_{\text{old, last day}}}{I_{\text{new, first day}}}$$

In our example, the old system yielded a score of 750 and the new system yields a score of 1,250. To scale down the new score to maintain continuity, we multiply the new score by  $(750/1,250) = 0.6$ . All subsequent scores (1994, 1995, and so on) will also be calculated in the same manner and then multiplied by 0.6, until another addition requires the determination of another multiplication factor.

One disadvantage of this method is the loss of information concerning the original set of chemicals and facilities in the presentation of one indicator that integrates all scores. Even if the indicator publishes the scores associated with each set of chemicals, the scale will have changed, prohibiting direct comparison. (Compare this to the method where original and supplemental indices are both tracked.)

Another disadvantage is the misrepresentation of the behavior of the new set of chemicals and facilities. The TRI indicator is distinct from the Dow in a way that affects the applicability of this system. The Dow uses a few stocks to model the entire market and assumes that the behavior of these stocks reflects the general behavior of all stocks. This implies that substitution of one stock for another in the Dow fits conceptually with its purpose. The TRI indicator seeks to reflect the levels of risk to human health and the environment by including a subset of the universe of all chemicals and facilities. The behavior of risks posed by all chemicals and facilities cannot be said to match the behavior of the set of TRI chemicals and facilities. The inclusion in TRI focuses a facility's attention upon particular chemicals and presumably results in changes of releases of TRI chemicals by TRI facilities. By fitting the combined score of new and old TRI chemicals and facilities to the score of the old, we inherently assume that the new have experienced reductions in risk identical to the old. In truth, we have no way of knowing the past pattern of releases for new additions. Emissions may have not changed at all since these chemicals have not yet been targeted by TRI; on the other hand, emissions may have been reduced more than emissions of old TRI chemicals because the new chemicals may have already been regulated by certain EPA programs or by states, or companies may have reduced emissions voluntarily.

### **Normalization to a Base Level**

This method reflects the Do-Nothing approach except for taking necessary adjustments for the use of normalization. Instead of using the score resulting from a base year, base levels could be used, defined as the sum of the component scores at the first year that each list is added to the TRI Indicator. For example, upon the first addition to the TRI (combining the initial roster, list 1, and the addition, list 2), the indicator could be calculated as follows:

$$I = \frac{(S_1 + S_2 + \dots + S_m + \dots + S_n)_{\text{present year}}}{(S_1 + S_2 + \dots + S_m)_{\text{first year of list 1}} + (S_{m+1} + \dots + S_n)_{\text{first year of list 2}}}$$

where:

$S$  = each chemical-facility-media component score,  
 $n$  = total number of TRI chemicals,

$m$  = number of TRI chemicals in the first list, and  
 $m-n$  = number of chemicals added to the roster.

Following the example, the score for 1988 would be  $(1,000/1,000)*100 = 100$ . The following scores would be  $(950/1,000) = 95$ ,  $(850/1,000) = 85$ ,  $(800/1,000) = 80$ , and  $(775/1,000) = 77.5$ . In 1993, the score would be calculated as follows:

$$\frac{750 + 500}{1000 + 500} = 83.3$$

While this score represents an increase, it is not as drastic as using the simple sum method, and it can be explained to the public as resulting from the addition of TRI chemicals and facilities to the indicator. This equation can also be used to indicate relative percentages of the two different sets of chemicals and facilities ( $750/1,500 = 50$  for the original and  $500/1,500 = 33.3$  for the new). However, as with ratio adjustment, the original set cannot be said to have improved by  $(77.5 - 50) = 27.5$  points.

### **Variations on the Previous Methods**

Improvements in the way in which the smaller TRI chemical universe models the larger one would lead to more meaningful comparisons between the old and new indices. One way to improve this modeling ability is to employ data on the new chemicals for the period predating their addition to TRI. If we had the release data, we could calculate exactly how inaccurate the small TRI chemical universe was as a model and adjust it accordingly. Although these data will not exist except as part of a state inventory, we could approximate them through the correlation of releases of other chemicals. For example, if a facility reports the release of a chemical because of its addition to the TRI, it is very likely that the chemical had been released at that level all along. A rough approximation would be to look at changes in releases from that facility and then correlate the release of the new chemical in back years.

Yet another possibility is to combine more than one of the above examples. For example, it may be appropriate to maintain one "primary" indicator score while also maintaining "subscores" for each of the sets of TRI chemicals (i.e., the original set and each additional set). The main score could be calculated using the simple sum and normalized with the ratio adjustment each time an additional set of chemicals is added. The subscores could be calculated for each set of TRI chemicals using the normalization to a base year; each of these subscores could be maintained separately. In our example, after the addition of chemicals, the main indicator score would be 750 while the subscores would be  $(750/1,000) = 75$  and  $(500/500) = 100$ . As in the discussion of the creation of separate indices, this combination depends upon the addition of TRI chemicals in large groups every number of years. If routine additions occur, the main indicator could be calculated as above and only one subscore, that of the original set of chemicals, could be maintained.

### **Start Over**

The last system that may be used is to announce the beginning of a new indicator. Once every 5 years the Agency could integrate all of the additions to and deletions from TRI that had occurred since the beginning of the previous indicator. EPA could announce that to better assess the risks to the environment posed by chemical releases, certain chemicals have been deleted or added based upon TRI criteria and that a new indicator, calculated in the same manner at the same scale, has begun. It is also quite possible that experience with the indicator may suggest a new mode of calculation by the time more chemicals and facilities are ready to be added.

## **Appendix H**

### **Additional Exposure Scenarios**

It has been suggested that the TRI Indicator be expanded to include additional exposure scenarios. These scenarios result from either the direct exposure to TRI chemicals or exposure to an indirect effect of the chemicals. A primary example of another direct exposure not currently incorporated into the indicator is the deposition of airborne chemicals into other pathways, such as groundwater. The most renowned examples of indirect exposures include the greenhouse effect, acid rain, the ozone "hole," and smog.

Since each of these scenarios poses a level of risk to human health and the environment, it would seem necessary to include them in an indicator which measures risk. However, the complexity of and uncertainty in modelling these scenarios makes direct insertion into the Indicator extremely difficult. The following endpoints are discussed for their potential inclusion into the TRI Indicator, the creation of a separate indicator for the endpoint, or difficulties in accomplishing either.

### *Global Warming*

Some of the TRI chemicals are considered "greenhouse gases." These chemicals, when released into the atmosphere, can absorb infra-red radiation which the earth emits as it establishes radiative equilibrium with the solar system. The potential result of this "effect" is the increase of the average temperature of the earth's surface, an increase which could lead to higher sea levels, droughts, floods, and climate changes.

The quantification of these risks is a hotly contested topic in academic, political and industrial circles. The temperature rise has been predicted to be anywhere between zero and eight degrees Celsius. The direction of the climate change resulting from the accumulation of greenhouse gases can be offset by natural occurrences such as volcanic eruptions or the appearance of El Niño, a circulating body of abnormally warm water in the Pacific Ocean. Since the results of the buildup of greenhouse gases have not been, and quite possibly cannot be, quantified, it is impossible to assign a greenhouse effect risk to the unit emission of a greenhouse gas. Thus the greenhouse effect cannot effectively be incorporated into the TRI Indicator.

This is not to say that the release of greenhouse gases, and their relative threat, cannot be traced with a separate indicator. In attempting to quantify the climate change potential associated with gaseous emissions, greenhouse gases have been weighted relative to their capacity to absorb infra-red radiation and their half-life in the atmosphere. These weights have been normalized to CO<sub>2</sub>, the greenhouse gas greatest in both presence in the atmosphere and rate of addition to the atmosphere. The other major greenhouse gases are listed below:

<u>Trace Gas</u>	<u>Lifetime (Years)</u>	<u>Global Warming Potential (Integration Time Horizon)</u>		
		<u>20 yrs.</u>	<u>100 yrs.</u>	<u>500 yrs.</u>
Carbon Dioxide	(120)	1	1	1
Methane	10	63	21	9
Nitrous Oxide	150	270	290	190
CFC-11*	60	4500	3500	1500
CFC-12*	130	7100	7300	4500
HCFC-22	15	4100	1500	510
CFC-113*	90	4500	4200	2100
CCl <sub>4</sub> *	50	1900	1300	460
CH <sub>3</sub> CCl <sub>3</sub>	6	350	100	34
CF <sub>3</sub> Br	110	5800	5800	3200
CO	<1	7	3	2

\* - TRI Chemical

Source: IPCC, 1990.

The emissions of greenhouse gases can be reported by their relative weight of contribution to the greenhouse effect and reported in a simple indicator.

### *Acid Rain*

Acid Rain results from the deposition of sulfur- and nitrogen- containing compounds, particularly sulfur dioxide and nitrous oxides, into clouds. The sulfur and nitrogen react with the water to form sulfuric and nitric acid which then accompany water during precipitation, leading to corrosion of structures and reductions in the pH of soils and water. Some researchers have attributed the elimination of habitat in different parts of the world to acid rain, particularly in areas where coal provides the primary energy source for combustion processes.

Like the greenhouse effect, it is extremely difficult to determine the effect caused by the unit emission of an "acid rain" chemical. The amount of sulfur and nitrogen which may combine to form an acid depends upon equilibrium concentrations in the area of concern. Although the acidity of sulfuric acid and nitric acid may be compared directly by their respective pH at a given concentration, and although the number of sulfur or nitrogen atoms present in a compound may determine the ability of a chemical to contribute to the creation of these acids, site-specific conditions will determine the quantity and concentration of the acids.

Like the risks associated with global warming, the risks posed to human health and the environment have not been quantified in terms of individual toxic risks. Some work has been done on health conditions and

respiratory problems. However, most work concerning acid rain has focused on population-based economic risks, a different perspective than the one used to determine the TRI indicator. The health effects seem to have been precursors to determining factors such as days lost at work and other economic inputs.

### *Stratospheric Ozone Depletion*

The depletion of the stratospheric ozone layer results from the reaction of chlorine and fluorine atoms in chlorofluorocarbons with ozone, breaking the ozone down into diatomic oxygen and oxygenated compounds. Since ozone absorbs incoming ultraviolet radiation, the deterioration of the ozone layer is resulting in dramatic increases in environmental exposure to UV radiation. This high-energy end of the spectrum has been shown to cause cataracts, suppress the immune system and induce cancer in humans. It has also been shown to adversely affect plant and animal life. Thus the risks to humans could lie anywhere from actual health hazards to loss of agriculture.

A major project at EPA, in conjunction with ICF, focused on determining the risks associated with CFCs and their alternatives in order to formulate policy options. The model tracks emissions into the atmosphere, models the reduction in the ozone layer, and calculates risks and damage associated with skin cancer, cataracts, aquatic impacts, crop loss, immunosuppression, and even a qualitative assessment to the food chain (starting with oceanic plankton). The model is complicated but could be used to determine risks associated with the emissions of CFCs.

A weighting scheme has been developed to determine the effectiveness of different CFCs at depleting the ozone layer. These weights are detailed below:

<u>Substance</u>	<u>Domestic 1986 Use</u> (millions kg)	<u>Weight</u>	<u>Weighted Production</u>
CFC-11*	91.3	1	91.3
CFC-12*	146.2	1	146.2
CFC-113*	71.1	0.8	56.9
CFC-114*	4.1	1	4.1
CFC-115*	4.61	0.6	2.8

\* - TRI Chemicals: Chlorinated Fluorocarbons are a category in the TRI.

Source: U.S. EPA (1987)

A separate indicator could be managed for ozone depletion through the use of these weights.

### *Tropospheric Ozone*

The creation of tropospheric (low atmosphere) ozone, one of the main constituents, results from the reaction of a radical oxygen atom with an oxygen molecule. This maverick oxygen atom is produced when ultraviolet radiation in sunlight breaks apart a nitrogen dioxide atom into nitrous oxide and oxygen. In normal circumstances, the ozone will react with the nitrous oxide in order to reform the nitrogen dioxide and the diatomic oxygen, the preferred state of being. However, the presence of volatile organic compounds (VOCs) in the air prevent this elimination of ozone by reacting with the nitrous oxide, creating nitrogen dioxide before the molecule can react with ozone. Thus it is the presence of both NO<sub>x</sub> and VOCs which lead to the formation of ozone in the troposphere.

The presence of ozone in the troposphere poses human health and environmental risks since it is this level of the atmosphere in which we live. Ozone causes respiratory ailments, particularly in the older and younger populations, and is an eye irritant.

The difficulty with pinning down the effects of emissions of either nitrous oxides or VOCs is their dependence upon one another for the creation and destruction of ozone. Rural and urban areas will have different impacts from increased or decreased emissions of VOCs. Some work has been done in modelling ozone formation at ORD, and these models can be consulted.

### *Particle Deposition*

Particle deposition differs from the volatilization pathway currently analyzed in the TRI indicator by tracing airborne emissions through exposure scenarios other than inhalation. Particles can land on clouds and precipitate, entering water bodies and exposing populations through drinking water. Particle deposition can also produce risks to wildlife through direct ingestion.

Many models have been developed at ORD to determine the exposure posed by particle deposition. The office would need to be contacted in order to consider the exposure scenarios which these cover.

## **Appendix I**

### **Description of the Computer Program**

This appendix describes the computer algorithm and the mathematical exposure modeling used to calculate the indicator elements. The computer algorithm used to calculate the TRI Environmental Indicators can be thought of as a three-part process; input, exposure modeling, and element calculation. First, we describe the fundamental data input files common to all of the element calculations. Next, we provide a step-by-step description of how these data files are linked with mathematical models and the exposure and toxicity weighting matrices in order to calculate the elements. The step-by-step description also delineates the mathematical steps used to model exposure and discusses the format and content of additional data files that are specific to the analysis of particular release pathways. A summary of the step-by-step process of computation is provided in Appendix G. Overall computation is replicable and verifiable, since it is performed completely within one computer program.

### **Programming Language and General Data Input**

Before we begin to construct an algorithm for indicator calculation, we must first select a programming language in which to implement the algorithm. We use the Statistical Analysis System (SAS). SAS is a data management and analysis programming language widely used in government and industry. In fact, an outstanding TRI analysis system, TRIPQUIC, uses SAS code to provide a rich set of exploratory tools. Its flexibility and power are unsurpassed among major data management systems. The choice to use SAS allows greater control of the input and output sequences and easily allows virtually limitless views of an indicator's make-up.

To support the calculation of the indicators, we created or used a variety of data files.<sup>1</sup> The program accesses these data files to obtain model input parameters as the models are run. All of the TRI Environmental Indicators calculations rely on three major data input files. First, the RELEASE<sup>2</sup> file contains information on releases for each facility-chemical combination in the TRI data base. The RELEASE file contains values for releases to all media and is the core of the indicators calculation. Emissions data can be presented as numerical point estimates, or, if releases are below 1,000 pounds, as an estimated range of emissions. To produce a conservative estimate of exposure potential, we will use the upper bound of the range as our estimate of emissions, since this value is the maximum that the facility could be emitting. Because the TRI database is continually updated and so fluctuates over time, we will use data from the two week period each year when EPA freezes the database for analysis. At that time all data for previous years are re-calculated in the model to accommodate revisions in the reported information. In the input process, data will be checked for errors and, if possible, corrected (if errors cannot be addressed, the data is flagged and the associated records are not scored with the model). Variables essential to the Indicator calculation that are contained in the file are listed below.

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<sup>1</sup>We refer to data files by a capitalized one word file name. This is only for clarity in the discussion; the actual locations and names of files appear in footnotes.

<sup>2</sup>Text file - TRIS.PROD.CHEMICAL.FILE89. This file was created to assist in creating the TRI National report. The entire file format is available from EPA.

Variable	Comment	Variable	Comment
TRI_ID	Unique facility identifier	ACTFLAG	Activity/use flags
DCN	Identification number used for matching facility with data in other data files	FUGAIR	Fugitive air emission of chemical from the facility (pounds per year)
ZIPCODE	ZIP code of the facility	STKAIR	Stack air emission of chemical from the facility (pounds per year)
NPDES	NPDES permit number of the facility	WATER	Direct water discharge emission from facility (pounds per year)
LATITUDE	Latitude for facility	LAND	On-site land release from facility (pounds per year)
LONGITUDE	Longitude for facility	UI	Release from facility to underground injection (pounds per year)
SIC	SIC code of facility	POTW	Discharge of chemical from facility to POTW (pounds per year)
CAS	CAS number of chemical	TRANSFER	Transfer of chemical off-site from facility (pounds per year) (other than POTW discharges)
TRIRCRA	RCRA ID number of TRI facility (if it has one)	BASIS1-BASIS5	Basis/method for estimating the quantity of release (separate variable for each type of release)

The ACTFLAG variable indicates how the chemical is used at the TRI facility. Although this variable has no direct role in indicator calculation, it will be useful for performing diagnostics on the indicators. Similarly, the method for estimating the quantity of the release is included as the variable BASIS and can be used for performing diagnostics on the indicators.

The second fundamental input file is the BGREACH file, which contains information on the populations and geographies of areas surrounding TRI facilities.<sup>3</sup> The BGREACH file was inspired by the current efforts to develop a GIS (Geographic Information System) at EPA. The file is a two-dimensional digital representation of the United States. As seen in Figure 1, the country is divided into 1 kilometer square cells.<sup>4</sup> For each of these cells, a variety of geographical information about the location can be stored. Storing information in this manner allows us to access all of the relevant geographical information for each TRI facility

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<sup>3</sup>FBXTRIS.TRIDENT.BGREACH - This file is a SAS housed on the EPA mainframe developed for this project.

<sup>4</sup>The choice of 1 kilometer is somewhat arbitrary. The size of each square can be set to any value. However, halving the length of one side of a square quadruples the size of the file.

by simply accessing the BGREACH cell that matches the location of the facility. This approach has significant advantages over having to access a number of different data files to retrieve different pieces of geographical information. Although the BGREACH file is not an exact reproduction of the geography and demographics of the U.S., it is a reasonably good approximation for our purposes. The variables contained in the BGREACH file are listed below.

Variable	Comment	Variable	Comment
CELLXY	Cartesian location of the cell	FLOW	Water volume (million liters per day)
POP	Population in the cell	WATERPOP	Population at intake
NEARSTAR	Nearest Weather Station ID	FIPS	State-County FIPS Code
WELL	Well density in cell	NEXTXY	Next cell for stream

Other variables can be added to the file if necessary. To build the BGREACH file, we extracted data from a variety of sources. Enumerated below are explanations of each variable, sources used to obtain data on the variable, and the weaknesses of each variable.

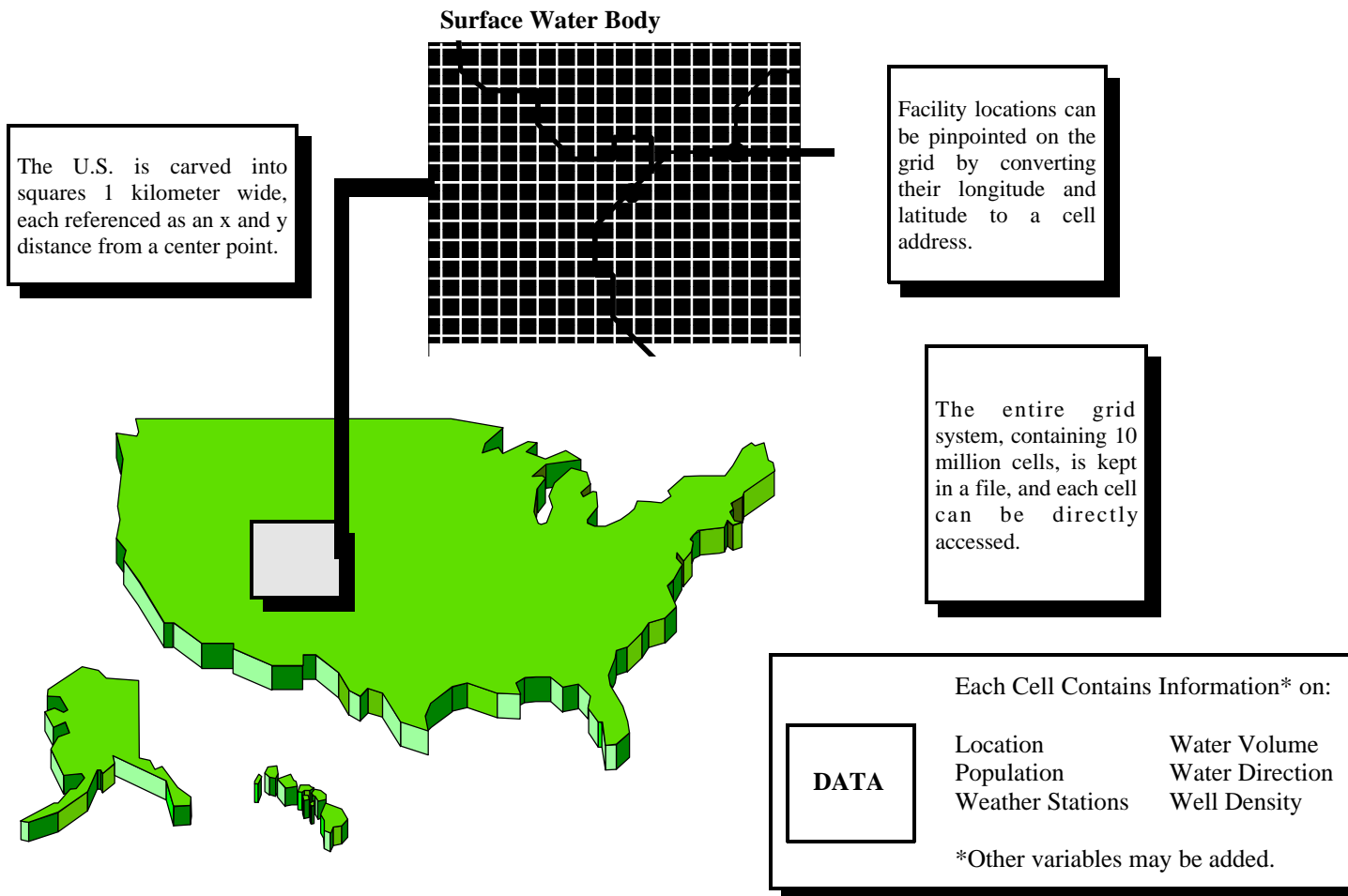
1. CELLXY - This value describes the relative location of the cell on the grid. This variable is the basic identifier that is used to link the information in BGREACH file with information from the RELEASE file and other data files. We link BGREACH to the RELEASE data by using the latitude and longitude data of the TRI facilities. To link the location of a TRI facility to a CELLXY value, the equivalent cartesian (x and y) distances of the TRI facility latitude and longitude are first calculated from a central point in the continental United States (96 degrees longitude and 37 degrees latitude). After these distances are calculated, a cell address can be directly calculated as follows:

$$Cell_{xy} = (y+1600) \cdot 10^4 + (x+1600)$$

where

Cell<sub>xy</sub> = cell address or location file,  
y = north/south distance (km) to center of US, and  
x = east/west distance (km) to center of US.

Adding 1600 (km) to the x and y distances guarantees positive values.



**Figure 1. How the TRI indicator program views the United States**

2. POP - This variable represents the number of people living in the cell. Information on populations were extracted from the Census Bureau's Block Group/Enumeration District (BG/ED) file. The BG/ED file reports population and longitude/latitude pairs for centroids of Block Groups and Enumeration Districts.<sup>5</sup> Each centroid was converted into a cell address ( $Cell_{xy}$ ) based on the above equation. Populations with equivalent cell addresses were summed. This exercise yielded a population number for each inhabited square kilometer in the United States.

One problem in this approach is that the land area of rural districts can be larger than a square kilometer. These areas are treated the same as a city block. In other words, a cell in the BGREACH file may contain a population that is actually spread over several kilometers. One way to adjust for this is to assume a uniform population distribution and allot populations to surrounding cells based on the reported size of the Enumeration District. However, since we propose in our methodology to set populations to a minimum value of 1,000, and since the population in an Enumeration District is usually less than 1,000, uniformly distributing populations is not necessary.

3. NEARSTAR - This variable identifies the location of nearby weather stations. It contains an identification value for the nearest weather station from the STAR (STability ARray) database. Using this identification number, the most probable prevailing weather conditions can quickly be fetched from a companion weather data file.

4. WELL - Variable WELL is a percentage of cell occupants who receive their drinking water from groundwater sources. It comes from a National Well Water Association (NWWA) county level file with counts of persons and homes either having private wells or receiving water from a utility that uses groundwater as its source. The NWWA file is catalogued using state and county FIPS codes. To insert these data into our BGREACH file, we first matched the FIPS codes to the Census BG/ED data. We then matched the BG/ED data to the cell identifier (CELLXY) as described above.

5. FLOW - This variable contains the flow volume of the surface water body in the cell. We obtained data on the continental stream network from the REACH file which is part of the Routing and Graphical Display System (RGDS). The stream network was mapped onto the BGREACH grid system based on longitude and latitude coordinates of stream segments in the REACH file. Since segment lengths are often larger than our 1 km grid network, care was taken to assure consecutive segments align within our grid. Essentially, the path of a surface water body was tracked at 1-km intervals instead of the multiple mile intervals in REACH. This did not increase precision, however, since each grid cell that is part of a stream segment will contain the flow properties of the segment itself in million liters per day.

6. WATERPOP - This variable contains the size of the population served by a drinking water utility that has an intake within the cell's boundaries. Using this variable, we are able to estimate the population exposed to chemicals in surface water in that cell. Data on the population served by drinking water utilities was derived from FRDS.

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<sup>5</sup>Block Groups and Enumeration Districts are terms used by the Census Bureau to describe very small units or blocks within metropolitan areas and rural areas generally containing not more than 800 people.

7. NEXTXY - This variable contains the address of the cell into which the surface water body flows next. It is the link that allows us to follow the movement of chemical discharges through the surface water network.

The final fundamental input data file is the TOX file. This file contains chemical-specific toxicological and chemical properties data. These data are linked via the chemical's CAS number to the RELEASE file and another data file.<sup>6</sup> The variables contained in the TOX file are listed below.

Variable	Comment	Variable	Comment
CAS	CAS number	AQNOAEL	Life cycle or chronic No Observable Adverse Effect Level for aquatic life
WOE	EPA cancer WOE category	LOGKOW	Log of the octanol water partition coefficient
		SOL	Water solubility (mg/l)
QSTAR	Cancer potency estimate (kg-day/mg) WOE	AIRDECAY	Decay rate in air (hr <sup>-1</sup> )
		WATERDECAY	Decay rate in water (hr <sup>-1</sup> )
RFD	Reference dose (mg/kg-day)	KOC	Soil-water partition coefficient
		POTWREMOVE	POTW removal efficiency
		POTWVOL	Percent of chemical that volatilizes at the POTW
LOAEL	Lowest Observable Adverse Effect Level (mg/kg-day)	POTWSLUDGE	Percent of chemical that partitions to sludge
NOAEL	No Observable Adverse Effect Level (mg/kg-day)	POTWDEG	Percent of chemical that degrades in the POTW
MED	Minimum effective dose (mg/kg-day)	DRE	Removal efficiency for municipal waste incinerator

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<sup>6</sup>FBXTRIS.TRIDENT.TOX.PHYSCHEM - SAS file housed on the EPA mainframe. This file will also be available in dBase III and Lotus 1-2-3.

Variable	Comment	Variable	Comment
LC50	Lethal concentration, 50 percent (concentration lethal to 50% of test organisms)	HC	Henry's Law constant
AAWQC	Acute Ambient Water Quality criteria or Ambient Aquatic Life Advisory Concentration	MW	Molecular weight
CAWQC	Chronic Ambient Water Quality Criteria or Ambient Aquatic Life Advisory Concentration	BCF	Bioconcentration factor

Chapter IV of the methodology describes the meaning and the sources of information for some of these variables. In addition, Appendix D presents the values for some of the TOX file variables for many of the TRI chemicals. In this section, we discuss the mathematics behind modeling exposure for each of the following exposure pathways: (1) stack and fugitive air releases, (2) direct surface water releases, (3) on-site land releases, (4) releases to POTWs, and (5) off-site transfers. We also outline the mechanics of combining the data files described above with (a) the mathematical equations that predict exposure and (b) with the weighting schemes used to derive the toxicity and exposure potential weights. The final facility-chemical-medium-specific element is the product of the toxicity weight, exposure weight and estimated population size in the case of the human health chronic indicator. The ecological indicator is the product of the toxicity and exposure weights.

The following discussions of exposure modeling frequently mention concentration and surrogate dose. We do not mean to imply that we somehow supplanted the risk assessment process and can accurately calculate cases. We speak of those terms only in the abstract. The method is a simple way to gauge relative risks from releases to different media in a congruent, defensible way. In some cases, the modeling will be purposely simple, given our lack of site-specific data. The differences in the level of refinement of exposure modeling are addressed by using the uncertainty weighting scheme discussed in Chapter IV.

#### Stack and Fugitive Air Releases

Ideally, reported stack and fugitive air releases from the TRI database would be modeled using site-specific data (such as source area or stack height). Since TRI does not contain such facility-specific information, we must use default values to model TRI facilities with established EPA air dispersion models.

For this methodology, we will use the Industrial Source Complex Long Term (ISCLT) model developed by the Office of Air Quality Planning and Standards (OAQPS). ISCLT is a steady-state Gaussian plume model used to estimate long-term pollutant concentrations downwind of a source. The concentration

is a function of site-specific parameters (stack height, stack velocity) and chemical specific decay rates.<sup>7</sup> To use the model, facilities directly releasing to air are first located on the BGREACH grid. Emissions rates in pounds per year are directly converted to grams per second by the following equation:

$$Q = \frac{453.6 \ q}{31,536,000}$$

where

Q = pollutant emission rate (in g/s), and  
q = pollutant emission rate (in lb/yr).

These emissions rates are then used in the following equation that determines the concentration at a distance  $r$  greater than 1 meter away from a point source<sup>8</sup>:

$$C_{air,r_{ijk}} = \frac{2K}{\sqrt{2\pi} \ r\theta} \cdot \frac{Q \ f \ S \ V \ D}{u\sigma_z}$$

where

$C_{air}$  = concentration at distance  $r$  ( $\mu\text{g}/\text{m}^3$ ),  
Q = pollutant emission rate (g/s),  
f = frequency of occurrence of wind speed and direction,  
 $\Theta$  = sector width (radians),  
S = smoothing function used to smooth discontinuities at sector boundaries,  
u = mean wind speed (m/sec),  
 $\sigma_z$  = standard deviation of vertical concentration distribution (m),  
V = vertical term (m),  
D = pollutant-specific decay in air ( $e^{\text{distance} \cdot \text{decay coefficient} / \text{wind speed}}$ ), and  
K = scaling coefficient for unit agreement.

The data in the BGREACH file are used as inputs to the ISCLT model equations. In addition, for each facility in the TRI data set, a stack height of 10 meters is assumed and ring radii from 50 meters to 50 kilometers from the source are specified. Stability Array (STAR) weather data are used to approximate typical wind speed and

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<sup>7</sup>Importantly, chemicals with extremely short half-lives in air will not be modeled using these procedures. Such chemicals will be assumed to degrade before significant exposure occurs. Products of decay could also be modeled where data permit.

<sup>8</sup>This equation is from EPA (1992). The equation is for a specific wind speed, direction, and category ( $ijk$ ). Each facility has several combinations of these that must be added to arrive at a total concentration at that point. The equation for area sources is similar.

direction around a given source. The weather data are stored in the STAR<sup>9</sup> data file and described in the table below.

Variable	Comment	Variable	Comment
ID	STAR Station ID	MEANWIND	Mean wind speed
LONGITUDE	Longitude of the station	CATEGORY	Stability category
LATITUDE	Latitude of the station	F1-F16	16 frequencies of occurrence

The NEARSTAR variable in the BGREACH file is matched with the ID variable in the STAR data file.

Based on the ISCLT equations, concentrations are calculated at each of the 100 cells (10 km x 10 km total area) nearest to the facility. These concentrations are then weighted by the population in the cell to derive a population-weighted average concentration over all 100 cells. If a cell contains no population, a value of 10 is used in the cell to assure that the population surrounding a facility is at least 1000 (i.e., there will be 100 cells with at least 10 persons in each cell). The program then combines the weighted concentrations with standard assumptions regarding inhalation rate and human body weight to arrive at a surrogate dosage:

$$DOSE = \frac{C_{air, avg} \cdot I_{air}}{BW}$$

where

DOSE = surrogate dose of contaminant (mg/kg-day),  
 $C_{air, avg}$  = population-weighted average air concentration (mg/m<sup>3</sup>),  
 $I_{air}$  = inhalation rate (m<sup>3</sup> per day), and  
 BW = human body weight (kg).<sup>10</sup>

Figure 2 graphically describes the air modeling portion of the indicator, and Table 1 lists the default parameters for ISCLT.

The program then uses the exposure weighting matrices (presented in Chapter IV for humans and aquatic life) to assign a weight to the calculated surrogate dose, either. For the air release pathway, we propose to use uncertainty category A to classify the air exposure potential (see Chapter IV discussion of exposure potential uncertainty).

Finally, the program accesses the TOX data file to assign a toxicity weight. The toxicity weighting matrix used by the program is presented in Chapter III. The product of the aquatic life exposure and toxicity scores yields an aquatic life indicator element for the facility-chemical-air release combination. For the human

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<sup>9</sup>FBXTRIS.TRIDENT.STAR - SAS file containing weather information used in air modeling. The file was converted to SAS for this project. It contains the same data used by ISCLT.

<sup>10</sup>This method uses the average adult body weight (male and female combined). for certain health endpoints (e.g., female reproductive effects), a different body weight value may be more appropriate (e.g., average adult female body weight).

health indicator, the exposure score, toxicity score, and the size of the population over the 100 cells are multiplied to yields an indicator element.

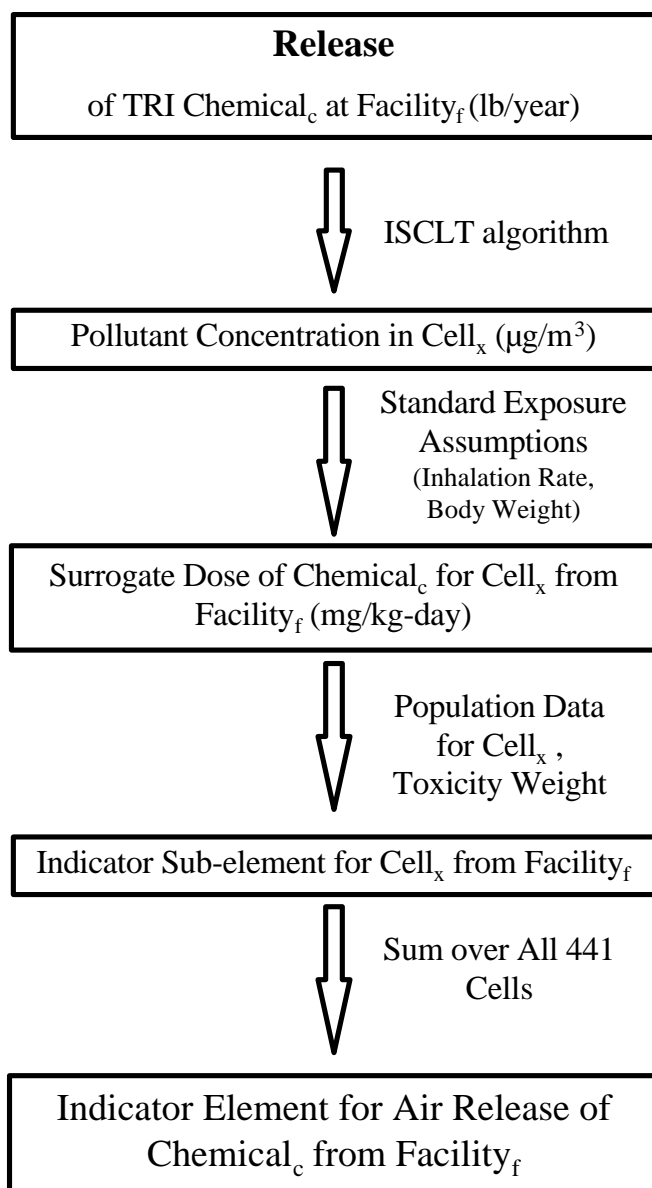
#### Direct Surface Water Releases

The Graphical Exposure Modeling System (GEMS) contains capabilities for estimating concentrations in surface water from direct chemical discharges (EPA, 1987a). We adopt GEMS data and methods for modeling surface water exposures. GEMS uses water volume data (from the GAGE database) and a routing database (the REACH database) that maps the path of the chemical to determine concentration. Another database Federal Reporting Data System (FRDS) is accessed to determine the populations at drinking water intakes.<sup>11</sup>

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<sup>11</sup>This database has a limitation in that it generally captures only those public systems that serve populations greater than 2500. Locations for community systems serving smaller populations are sporadically available.

**Figure 2. Calculation of Surrogate Dose and Indicator Element from Stack and Fugitive Air Releases**



**Table 1. Air Modeling Parameters**

Parameter	Value	Source/Comment
Stack height	10 m	EPA (1992)
Exit velocity	0.01 m/s	EPA (1992)
Stack diameter	1 m	EPA (1992)
Exit gas temperature	293 K	EPA (1992)
Area source size	10 m <sup>2</sup>	EPA (1992)
Area source height	3 m	EPA (1992)
Decay rate	varies by pollutant	
Body weight	70 kg	EPA Exposure Factors Handbook (EPA, 1990); value is for adults; lifetime age-weighted average (male and female combined) is about 62 kg
Pollution emission rate	site-specific	TRIS (lbs/yr)
Frequency of wind speed and direction	site-specific	STAR
Sector width	0.393 radians, or 22.5°	360° divided by 16 wind directions
Wind speed	site-specific	STAR (m/s)
Smoothing function	calculated	
Vertical term	calculated	
Population-weighted average air conc.	calculated	mg/kg-day
Inhalation rate	20 m <sup>3</sup> /day	EPA Exposure Factors Handbook (EPA, 1990)

GEMS uses a simple first-order decay equation along with volume and water speed estimates to calculate concentrations resulting from contaminant releases at a distance at time  $t$ . The general form is as follows<sup>12</sup>:

$$C_t = C_0 e^{-k_{\text{water}} t}$$

where

$C_t$  = concentration at time  $t$ ,  
 $C_0$  = initial concentration, and  
 $k_{\text{water}}$  = decay coefficient.

Using the REACH database, which contains information on the stream network of the United States, discharges are modeled as they make their way through the surface water network. Facilities are matched to appropriate streams using their latitude and longitude coordinates provided in TRI.

A facility discharging to water is located on the BGREACH grid. Using the water volume data contained in the BGREACH file, an initial concentration is calculated at the cell containing the facility. The surface water body network is stored in a separate file. The discharge from a facility is then matched to the grid cell containing the nearest surface water body. Then the surface water body is traversed and the concentration is adjusted along the water body.

This methodology considers two human health exposure pathways from surface water releases. First exposures from drinking water are calculated. As the pollutant passes through the stream network, concentrations at public drinking water intakes are noted. The population served (which is the variable WATERPOP in the BGREACH file) functions as the exposed population at that concentration. If a cell contains no drinking water intake, the WATERPOP variable is zero; otherwise, the WATERPOP variable is non-zero. The population-weighted water concentration is combined with standard exposure parameters to yield the following surrogate dosage:

$$DOSE = \frac{C_{\text{water, avg}} \cdot I_{\text{water}}}{BW}$$

where

DOSE	=	surrogate dose of contaminant (mg/kg-day),
$C_{\text{water, avg}}$	=	population-weighted average water concentration (mg/l),
$I_{\text{water}}$	=	drinking water ingestion rate (l/day), and
BW	=	human body weight (kg).

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<sup>12</sup>Chemicals with extremely short half-lives in water will not be modeled using this procedure. Such chemicals will be assumed to degrade before significant exposure occurs.

As with the air releases, the program then uses the exposure weighting matrix to assign an exposure weight to the calculated population-weighted surrogate dose. For the drinking water pathway, we propose to use uncertainty category B for exposure potential weighting for several reasons. First, the calculation of water concentrations does not consider partitioning of the chemical between the water column and suspended solids, deposition of the sediments along the water course, or other processes that may affect the fate and transport of contaminants along a surface water body. Furthermore, there is no consideration of the removal of contaminants during treatment of drinking water at the utility. All of these factors would tend to inflate the exposure potential evaluation.

Finally, the program accesses the TOX data file to assign a toxicity weight based on the toxicity matrix presented in Chapter III. The product of the exposure score, the toxicity score and the population for all of the cells with drinking water intakes yields a facility-chemical-drinking water element.

A second potential exposure pathway is from consumption of contaminated fish. Each segment of the affected water body may contain contaminated fish which could be caught and eaten by recreational fishers. As described above, the program tracks the concentration of the chemical as it traverses down the waterway; at each cell, the concentration in fish is derived by the following equation:

$$C_{fish} = C_{water} \cdot BCF$$

where

$C_{fish}$	=	concentration in fish, (mg/kg),
$C_{water}$	=	average water concentration in stream (mg/l), and
$BCF$	=	bioconcentration factor for chemical (l/kg).

Next, the fish concentration value is combined with standard exposure assumptions regarding fish consumption rates to determine surrogate dose from this pathway:

$$DOSE = \frac{C_{fish} \cdot I_{fish}}{BW}$$

where

$DOSE$	=	surrogate dose of contaminant (mg/kg-day),
$C_{fish}$	=	fish tissue concentration (mg/kg),
$I_{fish}$	=	fish ingestion rate (kg/day), and
$BW$	=	human body weight (kg).

The calculated surrogate dose in each cell is then weighted by the population of recreational fishers assumed to reside in that cell to yield a population-weighted average surrogate dose for all cells. The number of fishers is estimated as the total population in the cell times a fraction of persons who are assumed to fish for recreation. We derived state-specific fractions of persons who eat fish from state-specific fishing rates found in the 1991 National Survey of Fishing, Hunting, and Wildlife Associated Recreation (U.S. FWS, 1993).

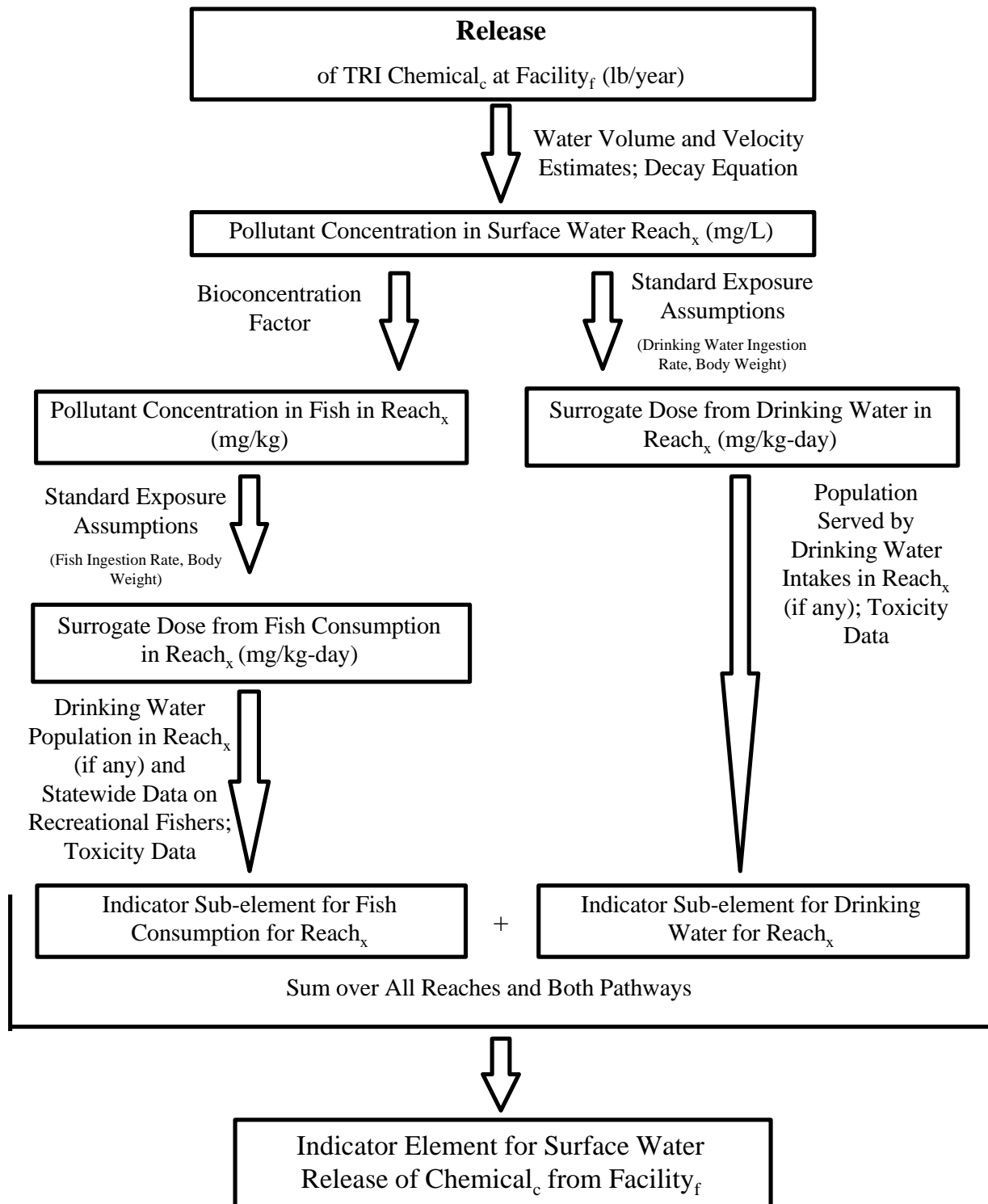
As with the drinking water pathway releases, the program then uses the exposure matrix to assign a weight to the calculated population-weighted surrogate dose. For this exposure pathway, we propose to use

uncertainty category C for exposure potential for several reasons. First, as with the drinking water pathway, the estimated water concentrations are probably an overestimate because we don't consider all processes in surface water that affect concentrations. Second, fish concentrations are actually dependent on the type of species, particularly its lipid content and its position in the food chain. Finally, the actual probability of recreational fishing in the particular stream reach being modeled is unknown, as is the actual quantity of fish consumed from that particular reach.

Next, the program accesses the TOX data file to assign a toxicity weight based on the toxicity weighting matrix presented in Chapter III. The product of the exposure score, the toxicity score and the population for all of the cells traversed by the contaminated surface water yields an element for the facility-chemical-fish ingestion combination.

Figure 3 shows our recommended surface water approach, and Table 2 lists model parameters for surface water modeling.

**Figure 3. Calculation of Surrogate Dose and Indicator Element from Surface Water Release**



**Table 2. Surface Water Modeling Parameters**

<b>Parameter</b>	<b>Value</b>	<b>Source/Comment</b>
Decay rate	varies by pollutant	
Dilution rate	site-specific	REACH (EPA, 1987a)
Water volume and velocity	site-specific	REACH (EPA, 1987a)
Population-weighted average water concentration	calculated	mg/L
Drinking water ingestion rate	2 liters	EPA Exposure Factors Handbook (EPA, 1990)
Body weight	70 kg	EPA Exposure Factors Handbook (EPA, 1990); value is for adults; lifetime age-weighted average (male and female combined) is about 62 kg
Average chemical concentration in stream	calculated	mg/L
Bioconcentration factor	varies by pollutant	L/kg
Fish tissue concentration	calculated	mg/kg
Fish ingestion rate	0.0065 kg/day	Exposure Factors Handbook (EPA, 1990)

## On-Site Land Releases

On-site land releases include releases to landfills, surface impoundments, land treatment units and underground injection. This section describes methods to evaluate exposure from these releases. For simplicity, the following discussion will focus on landfill disposal, but the same evaluation principles will apply to the other types of land releases, with the exception of underground injection<sup>13</sup>.

Two major pathways are considered for on-site land releases: chemicals may volatilize to air or leach to groundwater. Volatilization of chemicals from on-site landfills is reported under the fugitive emission estimate for the facility and is thus handled as a direct air release.

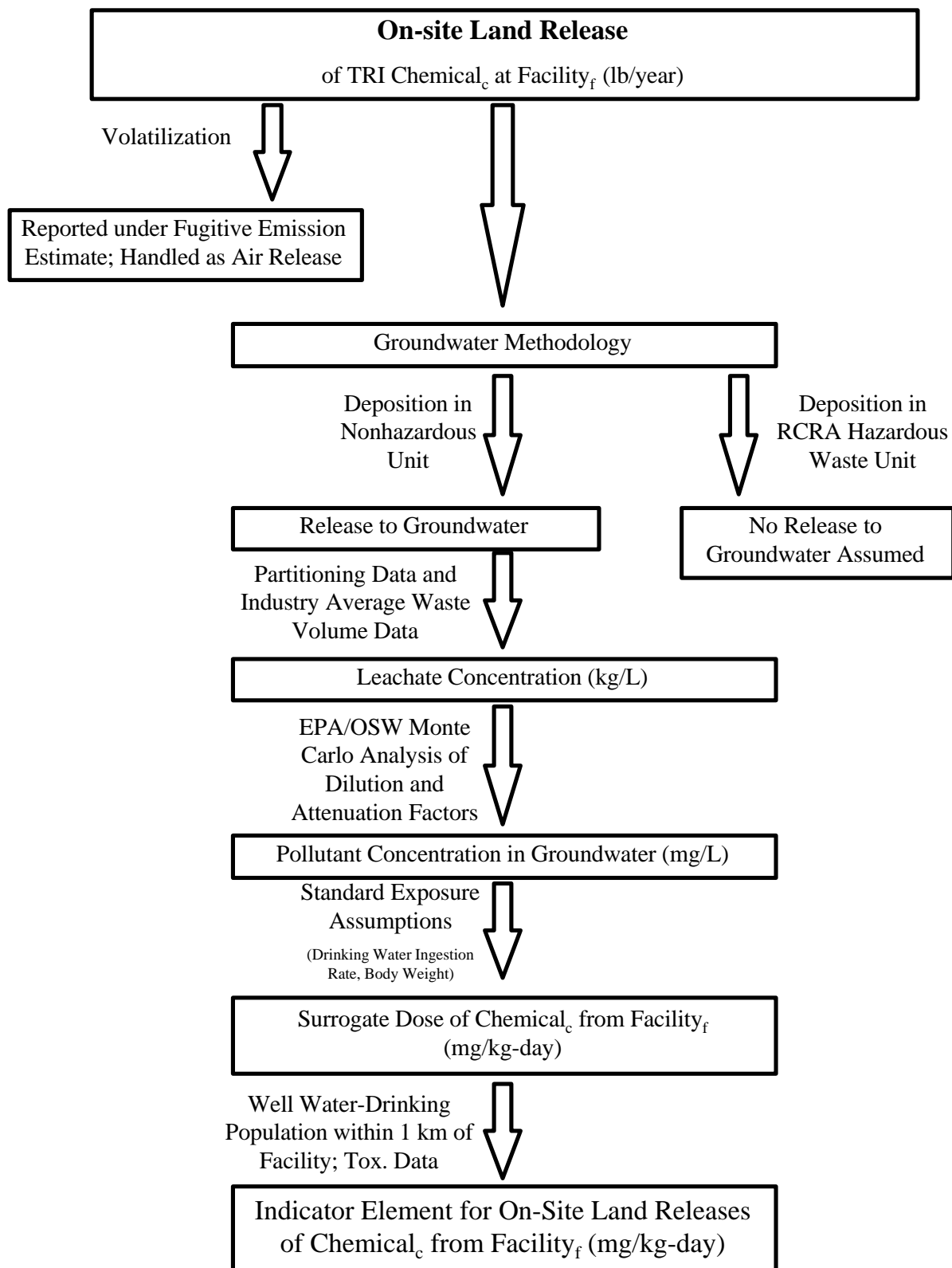
Groundwater contamination is also a concern for land releases. However, the modeling of groundwater releases will depend on the regulatory status of the unit in which the chemical is released. Chemicals could be deposited in an on-site RCRA-regulated hazardous waste unit, or in an on-site nonhazardous solid waste management unit. RCRA standards for hazardous waste units are, by regulation, designed to include technical controls to prevent release of contaminants into groundwater; if chemicals are placed in such regulated units, it will be assumed that releases to groundwater are negligible. If chemicals are placed in RCRA nonhazardous land disposal units, we will model the release of chemicals to groundwater. This analysis assumes that if the TRI form reports a RCRA ID number for the facility, then the on-site land releases are assumed to go to a RCRA regulated unit. Otherwise, the on-site land release is assumed to occur in a nonhazardous land disposal facility.

The TRI forms do not provide site-specific information that aids in the evaluation of groundwater transport, such as geohydrological data. Unfortunately, these data are extremely site-specific and are not amenable to characterization by state or region of the country. To maintain a concentration/exposure measure consistent with the approaches suggested for direct air and water releases, we propose an approach that gives a concentration at the exposure point (the well) to be combined with exposure assumptions to yield a surrogate dose. This approach requires two steps: estimating leachate concentration (a measure of the amount of chemical that partitions from the waste to water) and estimating the dilution and attenuation of leachate from the disposal site to the well location. The approach to evaluating exposure from landfilling is summarized in Figure 4.

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<sup>13</sup>The methodology proposes an alternate approach to evaluate exposure from underground injection of TRI chemicals. Under well-managed conditions, these facilities are designed to pose minimal risks to human health or the environment. However, certain conditions can lead to the failure of these facilities and the release of chemicals to human and environmental exposure pathways. An exposure analysis for these releases would have to include an evaluation of the likelihood of the failure as well as an evaluation of the exposure impacts of such a failure.

**Figure 4. Calculation of Surrogate Dose and Indicator Element from On-site Land Releases**



Leachate concentrations can be estimated using a modified modeling approach with chemical-specific parameters. The general form of this estimate is as follows:

$$C_l = \frac{C_s}{K_d \times B_d}$$

where

$C_l$	=	concentration in leachate (kg/l or $1 \times 10^6$ mg/kg),
$C_s$	=	concentration in landfill solids (kg/m <sup>3</sup> or 1000 mg/kg),
$K_d$	=	soil/water partition coefficient (l/kg), and
$B_d$	=	bulk density of material in landfill (kg/m <sup>3</sup> ).

This equation assumes that the landfill material essentially contains close to 100% solids. This assumption (and the equation) will have to be modified for use for surface impoundments. It must be noted that the concentration in the leachate,  $C_l$ , must be compatible with the chemical-specific solubility so that the smaller of the two values is used.

The concentration in the landfill solids,  $C_s$ , can be estimated by dividing the total mass of contaminant disposed (mg/yr) by the total mass of waste disposed in the unit each year:

$$C_s = \frac{M_c(\text{mg per yr})}{M_w(\text{kg per year})}$$

where:

$M_c$	=	total mass loading of contaminant to landfill (mg per year), and
$M_w$	=	total mass of waste disposed in landfill (kg per year).

The value for  $M_c$  is available in the TRI database; the value for  $M_w$  will be taken from EPA (1988a). This report summarizes the distribution (by number of facilities and by industry type) of the tons per year of waste disposed in industrial nonhazardous solid waste landfills. Data are also reported for surface impoundments, waste piles and land treatment facilities. These summaries are reproduced in Appendix F. This appendix was converted to a data file WASTE<sup>14</sup>, with the following content:

Variable	Comment	Variable	Comment
SIC	SIC code for which the waste volume is applicable	UNITTYPE	Type of management unit into which waste is placed
WASTEVOL	Industry-specific waste volume disposed per year		

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<sup>14</sup>FBXTRIS.TRIDENT.WASTE - SAS file containing waste volume information.

It should be noted that using  $M_w$  as the divisor in landfill concentration may underestimate the total concentration of the TRI chemical, since the landfill may include some of the same chemicals from sources other than TRI facilities.

A summary of the values used in the groundwater calculation and the sources of these values appear in Table 3.

**Table 3. Groundwater Modeling Parameters**

Parameter	Value	Source/Comment
Concentration in leachate	calculated	mg/L
Partition coefficient	varies by pollutant	

Once leachate concentrations are estimated, the next step is to determine the magnitude of dilution and attenuation of contaminants that occur as the contaminant travels from the source to the well. The Office of Solid Waste performed an analysis of dilution and attenuation of contaminants in groundwater during the development of the Toxicity Characteristic Leaching Procedure (TCLP) rulemaking (55 (61) Federal Register 11798). For that rule, OSW used Monte Carlo analysis to evaluate dilution and attenuation factors (DAFs) for 44 chemicals. In the Monte Carlo analysis, multiple iterations of a groundwater model were performed. For each model run, model parameter values were drawn randomly from their distributions. (It should be noted that distance to the well was one of the parameters varied in the analysis: the distribution of distance between a source and a well was derived from a survey of Subtitle D facilities). The result of the analysis was a distribution of model results, where each model result was a DAF. OSW then selected the 85 percentile DAF for use in its regulatory calculations. For most chemicals modeled, the 85th percentile dilution and attenuation factor was approximately a factor of 100. For this methodology, we will use the OSW 85th percentile dilution and attenuation factor of 100 to estimate groundwater concentrations at the well from land releases. The concentrations are then used to calculate surrogate doses. It should be noted that OSW's DAFs are not intended to reflect the effect of pumping in drinking water wells on the concentration of chemicals in groundwater, and thus calculation of TRI surrogate dosages are oversimplified.

The program then uses the exposure matrix to assign a weight to the calculated surrogate dose. For the groundwater pathway, we propose to use uncertainty category C, since the exposure estimate is based on a conservative, steady-state estimate of leachate concentration, and on a conservative, generic dilution and attenuation factor.

The program then accesses the TOX data file to assign a weight based on the toxicity matrix presented in Chapter III. The proposed population exposed to contaminated groundwater is calculated from the number of persons receiving drinking water from groundwater within 4 square kilometers of the facility. The population of persons served by well water is available for each county from the National Well Water Association data files. From these data, we can derive a "well water drinker" population density for each county. We will then calculate the population of well water drinkers within 4 km<sup>2</sup> of the landfill site as our exposed population. This value is included in the BGREACH file as the WELL variable. The product of the

exposure score, the toxicity score and the population over 4 km<sup>2</sup> yields an element for the facility-chemical-groundwater combination.

### Releases To POTWs

In 1988, 570 million pounds of TRI chemicals were discharged to the country's Publicly Owned Treatment Works (POTWs) compared with 360 million pounds discharged directly to surface waters. Modeling exposure from TRI discharges to POTWs requires consideration of (1) overall removal efficiencies of POTWs and resulting effluent discharges from POTWs and (2) residuals management at POTWs. A summary of our proposed approach to modeling POTW emissions is found in Figure 5.

To store POTW-specific information, we use a data file called POTW.<sup>15</sup> The appropriate POTW file is matched to the TRI transfer via the DCN (Document Control Number) variable in the RELEASE data file. Variables contained in the POTW file are shown below.

Variable	Comment	Variable	Comment
DCN	ID used for matching with TRI transferring facility	ZIPCODE	ZIP code of the POTW facility
BASIS6	Basis/Method for estimate of quantity of release to POTW	SLUDGE	Sludge disposal method employed by the POTW

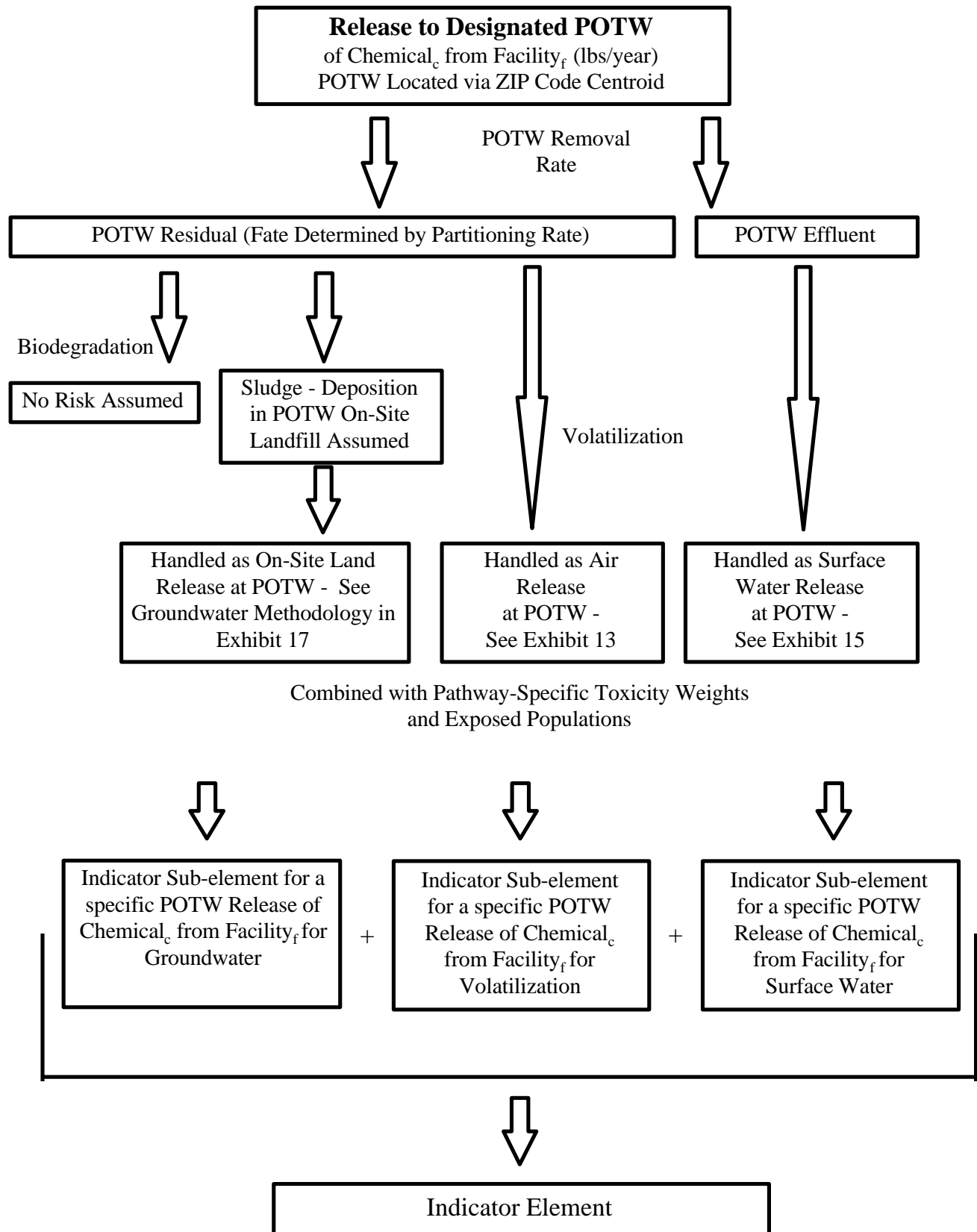
The ZIP code of the POTW is provided on the TRI form of the facility making the transfer. Using this data file, POTWs are located on the BGREACH grid based on the latitude and longitude of the ZIP code centroid. To do so, we must match the ZIP code centroid with a latitude and longitude. This information is stored in a data file called ZIPCODE.<sup>16</sup> The format of the ZIPCODE file is given below.

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<sup>15</sup>TRIS.PROD.POTW.FILE89 - This file is also part of the national report family of files. The full record layout is available from EPA.

<sup>16</sup>FBXTRIS.TRIDENT.ZIPCODE.CENTROID - SAS file containing FIPS, zipcode, longitude/latitude, and census information for all ZIP codes in the United States.

**Figure 5. Modelling of Exposure from POTW Releases**



Variable	Comment	Variable	Comment
ZIPCODE	ZIP code	FIPS	State-County FIPS CODE
LONGITUDE	Longitude of the ZIP code centroid	LATITUDE	Latitude of the ZIP code centroid
POP	ZIP code population		

Once we have located the POTW, the next step is to apply the overall POTW contaminant removal rate (stored in the TOX file) to the release.

POTWs are not completely effective at removing all of the chemicals in the influent; some of the chemical loading in the influent will be released in the POTW effluent. Typical overall POTW removal efficiencies vary by chemical. Chemical loadings that are removed by POTW treatment processes partition to several pathways within the POTW, including biodegradation, volatilization, and adsorption to sludge. Using average removal and partitioning rates, chemicals will be divided among effluent, biodegradation, air and sludge pathways. The Domestic Sewage Study (EPA 1986) gives both typical POTW removal efficiencies and within-POTW partitioning rates for many TRI chemicals. These values will be used in this methodology. Chemicals lacking partitioning rates will be assigned rates based on their chemical class. To do so, each chemical having partitioning rates in the Domestic Sewage Study will be assigned to a class (halo-organic, metal, etc.), and an average determined for each class. The average rate will be applied to other TRI chemicals in that class lacking specific partitioning rates.

This overall removal rate allows the program to calculate the loading of contaminant remaining in the POTW effluent and the loading that remains in the POTW. Contaminants remaining in the POTW are partitioned within the POTW, using partitioning rates stored in the TOX file. The partitioning rates allow us to estimate the amount of contaminant in the POTW sludge and in the POTW volatile emissions, as well as the amount that degrades.

Once the fates of chemicals entering the POTW are determined, the exposure levels associated with chemical loadings to each compartment will be estimated. Chemicals that escape in the POTW effluent will be modeled using the surface water evaluation methods described above. Since ZIP code centroids are used to locate the POTW, it is possible that a POTW may be placed on a BGREACH grid cell without a water body running through it. In this case, the water body receiving the POTW effluent is determined by finding the nearest water body to the ZIP code centroid. We could improve this estimate if we could find longitude and latitude information for POTWs from a source other than ZIP codes. Chemicals that biodegrade will be assumed to cause no further exposure. POTW volatilization releases will be treated like area-source air releases, as described above.

For chemicals that partition to sludge, the models used to depict exposure will depend on the sludge disposal method employed by the POTW. The remaining problem is to determine which POTWs engage in which sludge disposal practices since it cannot be determined from the TRI database. A database does exist (the National Sewage Sludge Survey) that describes the sludge disposal methods employed by POTWs in the United States. If we can identify methods used at specific POTWs from this database, the exposure levels from POTW sludge contaminants can be modeled using the same methods used to model direct releases of contaminants, depending on the POTW sludge disposal practice (incineration, landfilling, land application, etc.). For incinerated sludge, destruction and removal efficiencies from the TOX file are applied and then air

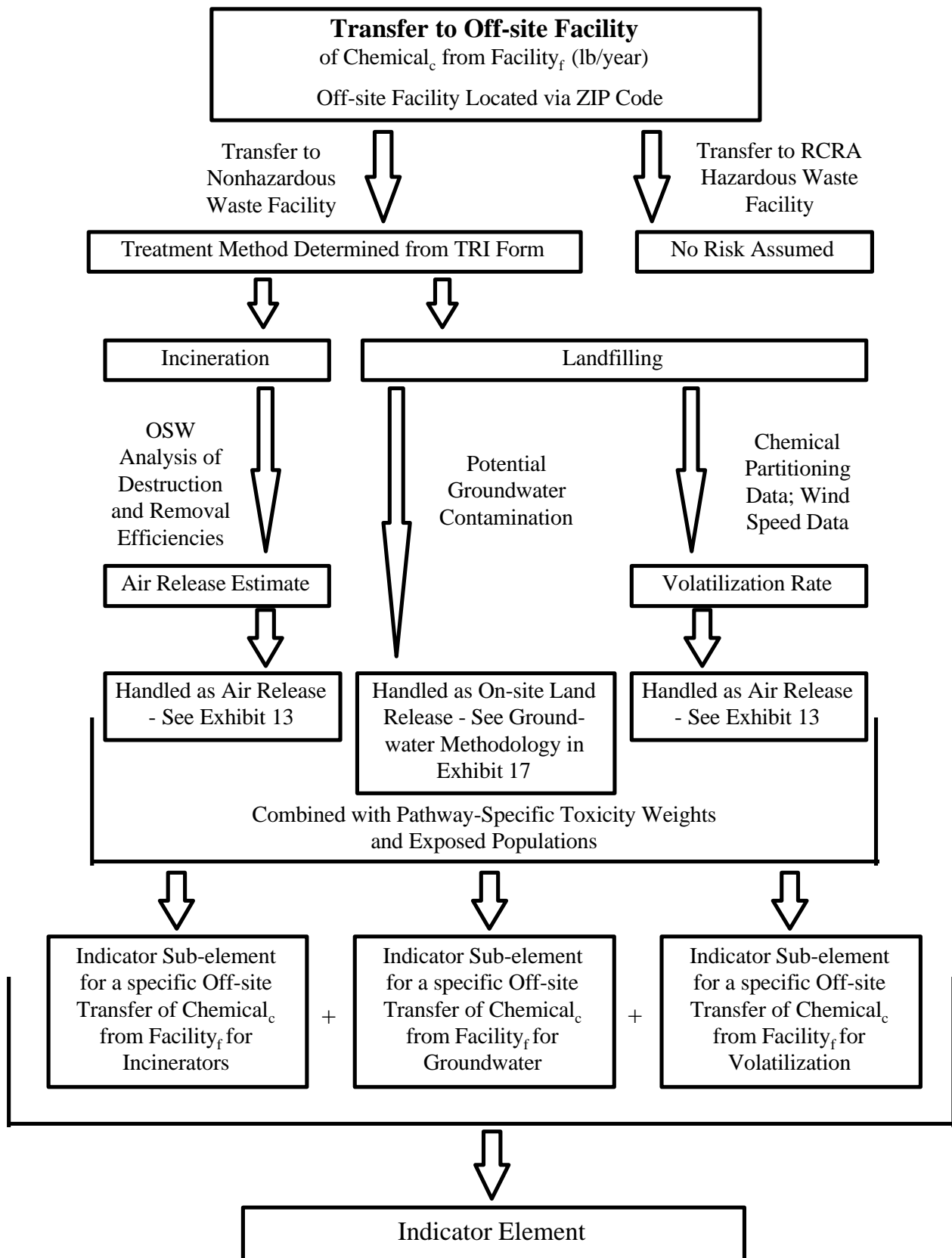
modeling is performed as described in the Air Releases section above. Land disposal of sludge can be modeled as a land release using methods described above. Populations surrounding the disposal facility or disposal area will be modeled as the exposed population. If extracting data on disposal practices is too cumbersome or if a match cannot be found, other methods for modeling these exposures will have to be adopted. One possible method is to use results from the national aggregate population risk assessment for municipal sludge performed in support of upcoming municipal sludge rules. From this risk assessment, we could obtain average exposures per ton of sludge disposed, by disposal method. These results could be used for this analysis by weighting these unit exposures by the amount of sludge disposed by each practice (either regionally or nationally), then multiplying by the tons of sludge disposed by the POTW (which can be estimated based on flow to the POTW).

The resulting sum of the uncertainty-adjusted, population-weighted surrogate doses from POTW effluent, volatilization at the POTW, incineration of sludge, volatilization of land disposed sludge, and groundwater contamination from land-disposed sludge are combined with the chemical-specific toxicity score to yield a facility-chemical-POTW release element.

#### Off-Site Transfers

In 1988, over 17 percent of TRI volume was transferred to off-site locations for storage or disposal. Figure 6 presents a summary of our proposed method to model off-site transfers. TRI reporters are supposed to supply the name and address of the receiving facility. From these data, we must determine if wastes are sent to a hazardous or nonhazardous waste management facility. Efforts are currently underway between OSW and OPPT to match facilities reported in TRI with RCRIS reporting to aid in making this determination. Chemical submissions indicating transfer to a RCRA hazardous waste facility will not be included in the indicator; for the purposes of simplifying the indicator calculation, these transfers are assumed to pose no further risk in a regulated disposal facility. Only transfers to nonhazardous facilities will be modeled.

**Figure 6. Modeling of Exposure from Off-site Transfers**



As with POTW transfers, to assess exposure potential associated with off-site transfers, we must have information on the off-site facility location and some of its characteristics. To store off-site facility information, we constructed the data file OFFSITE.<sup>17</sup> Variables necessary from the file are shown below.

Variable	Comment	Variable	Comment
DCN	ID used for matching TRI facility	RCRA-ID	RCRA ID number (if it has one)
ZIPCODE	ZIP code of off-site facility	BASIS7	Basis/Method for estimating quantity of chemical transferred off-site
TREAT	Type of treatment		

We match data in the RELEASE file to this file via the DCN (Document Control Number) variable. The ZIP code for the off-site facility to which chemicals are transferred is contained in the TRI data base. The ZIP code serves, in conjunction with the ZIPCODE data file, to locate our facility on the BGREACH grid, as was described for locating POTWs. It should be noted that OSW and OPPT are jointly working on a tracking system to match TRI releases to the RCRIS data base. If this effort is completed before we implement the TRI Environmental Indicator, we may be able to use the fruits of that effort for more precise tracking of the off-site releases. Once we have located the off-site facility, we also need to know (a) the regulatory status of the unit to which the material is transferred and (b) the treatment/disposal technologies used by the off-site facility. The regulatory status of the off-site units could be determined in a number of ways. The TRI form requires the reporting facility to give the RCRA-ID number of the off-site facility to which the chemical is being transferred. We could assume that if such a number is reported, then the chemical is being transferred to a RCRA-regulated unit. Otherwise, we will assume that it is a RCRA Subtitle D nonhazardous management unit.

The TRI forms also require the reporting facility to indicate the treatment/disposal method used at the off-site facility. Where this information is reported, it is stored as the TREAT variable in the OFFSITE data file; the method reported will be assumed to be the treatment/disposal method employed by the off-site facility. If this information is not reported (despite the requirement), we will have to assume a distribution of treatment/disposal methods, based on the frequency of treatment/disposal methods reported for that chemical practiced at nonhazardous Treatment, Storage or Disposal Facilities (TSDFs) where the treatment/disposal method is known. Using this distribution, we will assign the appropriate proportion of the release to each reported treatment/disposal method.

Once the treatment method is established, we model exposure potential using the methods described above. The exposure evaluation for off-site transfers will obviously depend on the type of treatment/disposal employed off-site. We are still investigating methods for evaluating exposures from various treatment and disposal technologies, including underground injection. We currently have methods to evaluate exposure from two offsite disposal technologies: waste incineration and landfilling.

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<sup>17</sup>TRIS.PROD.OFFSITE.FILE89 - This file is also part of the national report family of files. The full record layout is available from EPA.

Air releases from off-site nonhazardous waste incinerators can be modeled like direct air releases. We have obtained destruction and removal efficiencies (DREs) for nonhazardous waste incinerators from an OSW analysis of municipal solid waste combustion (EPA, 1987b); these values are included in the TOX data file. For inorganics, values are taken from multiple hearth sludge incinerator studies (EPA, 1993).

For landfills, two major pathways will be considered. The groundwater pathway will be modeled for off-site releases in the same manner as for on-site land releases. Volatilization, however, will be handled differently. For on-site releases, volatilization is included in reported fugitive emissions and thus exposure is modeled with air releases. For off-site land releases, volatilization emissions from land disposal must be estimated before exposure can be modeled. Since the volatilization rate is a function of vapor concentration, the vapor concentration must be calculated. This involves two steps: partitioning from the solid to the water, and then water to air. Simple steady-state relationships can be used to approximate these partitioning processes if certain chemical-specific data are known.

The equation for determining the concentration of chemical in the liquid phase (i.e., leachate) was given earlier in the "On-Site Land Release" section:

$$C_l = \frac{C_s}{K_d \times B_d}$$

where

$C_l$	=	concentration in leachate (liquid phase) (kg/l),
$C_s$	=	concentration in landfill solids (kg/m <sup>3</sup> ),
$K_d$	=	soil/water partition coefficient (l/kg), and
$B_d$	=	bulk density of material in landfill (kg/m <sup>3</sup> ).

The second calculation determines the vapor phase concentration from the liquid phase concentration using Henry's Law Constant (the ratio of the contaminant concentration in the vapor to the concentration in the liquid phase):

$$C_v = H C_l$$

where

$C_v$	=	concentration in vapor phase (kg/l) and
$H$	=	Henry's Law Constant (dimensionless).

Now that an equilibrium vapor concentration has been determined, the rate of volatilization may be estimated from a first-order rate equation:

$$Vol\ Rate = k_{vol} C_v$$

where

$k_{vol}$	=	volatilization rate constant.
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The volatilization rate constant is taken from a EPA (1985) equation for uncovered monofills:

$$k_{vol} = \frac{0.17 u (0.994)^{(T - 20)}}{\sqrt{MW}}$$

where

u = wind speed (m/s),  
T = ambient air temperature, assumed to be 15°C,  
MW = molecular weight (g/mol) and  
0.17 and 0.944 are empirical constants.

All of these formulae may be combined to express the volatilization rate as a function of the chemical concentration in the solid phase:

$$Vol Rate = \frac{0.17 u (0.994)^{(T-20)} H C_s}{k_d B_d \sqrt{MW}}$$

These volatilization emissions estimates, along with weather and data on populations surrounding the off-site disposal facilities, will be used to arrive at population-weighted concentrations in the same way as fugitive direct air releases from TRI facilities. Population data will be extracted using the zip code of the facility receiving the waste. Volatilization parameters are summarized in Table 4.

The resulting sum of the uncertainty-adjusted, population-weighted surrogate doses from incineration, volatilization and groundwater exposures are combined with the chemical-specific toxicity score to yield a facility-chemical-off-site transfer element.

**Table 4. Volatilization Modeling Parameters**

Parameter	Value	Source/Comment
$K_d$	varies by pollutant	Chemical properties database (Appendix D)
Molecular weight	varies by pollutant	Chemical properties database (Appendix D)
Henry's Law constant	varies by pollutant	Chemical properties database (Appendix D)
Average area of source: municipal solid waste landfill	32.5 acres	EPA (1988b)
Median area of source: industrial nonhazardous land disposal	landfill: 3 acres surface impoundment: 0.5 acres land treatment: 15 acres waste pile: 0.5 acres	EPA (1988c)
Mean wind speed	site-specific	m/s; from STAR data

### **Evaluating Exposure Potential -- Ecological**

The estimated ambient water concentration value is used directly to evaluate potential exposures to aquatic life. The method for evaluating ambient surface water concentrations resulting from TRI releases is discussed in Chapter IV of the methodology. Since the Chronic Ecological Indicator includes only one exposure pathway, there is no reason to use an uncertainty adjustment for cross-pathway uncertainty. Therefore, these surrogate values are used directly as the exposure potential weights for aquatic life.

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